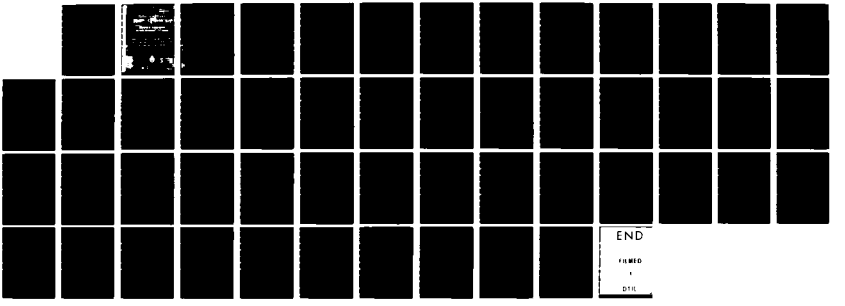
AD-A124 158 FINNIGAN BASIC COMPUTER PROGRAMS FOR THE ENTRY DISPLAY AND COMPACT STORAG.. (U) DEFENCE RESEARCH ESTABLISHMENT OTTAWA (ONTARIO) J G PURDON MAR 81 DREO-TN-82-2 1/1

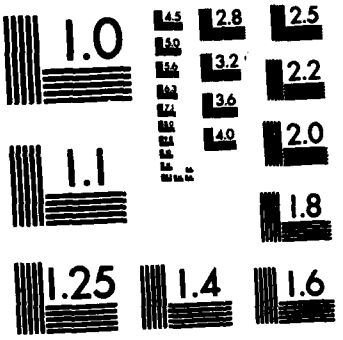
UNCLASSIFIED F/G 9/2 NL



END

FILMED

DTIC



# DEFENCE RESEARCH ESTABLISHMENT OTTAWA

DREO TECHNICAL NOTE NO. 82-2
DREO TN 82-2

# FINNIGAN BASIC COMPUTER PROGRAMS FOR THE ENTRY, DISPLAY AND COMPACT STORAGE OF MASS SPECTRA IN A FINNIGAN 6115 DATA SYSTEM

by

J.G. Purdon

**CAUTION**

This information is furnished with the express understanding that proprietary and patent rights will be protected.

RESEARCH AND DEVELOPMENT BRANCH

**DEPARTMENT OF NATIONAL DEFENCE**
**CANADA**

# DEFENCE RESEARCH ESTABLISHMENT OTTAWA

**TECHNICAL NOTE NO. 82-2**

# FINNIGAN BASIC COMPUTER PROGRAMS FOR THE ENTRY, DISPLAY AND COMPACT STORAGE OF MASS SPECTRA IN A FINNIGAN 6115 DATA SYSTEM

by

J.G. Purdon

Chemical Defence Section
Protective Sciences Division

**MARCH 1981**
**OTTAWA**

## ABSTRACT

Finnigan BASIC programs have been developed for the creation, compact storage and output of files containing mass spectra on a Finnigan 6115 Data system used with Finnigan 3000 and 4000 Series Gas Chromatograph/Mass Spectrometers. Entries can be made directly from the memory of the data system for spectra acquired on the specific instrument or from a keyboard for spectra obtained from external compilations. The resulting mass spectra can be stored both in Finnigan BASIC on magnetic tape permitting further BASIC operations and on magnetic disc in the computer for standard mass spectral manipulation by the operating system.



## RÉSUMÉ

Des programmes BASIC Finnigan ont été mis au point pour créer, mettre en mémoire et restituer des fichiers renfermant des spectres de masse dans un système informatique Finnigan 6115 utilisé avec des ensembles chromatographe gazeux/spectromètre de masse Finnigan, séries 3000 et 4000. Les valeurs peuvent être introduites directement à partir de la mémoire du système informatique, dans le cas des spectres recueillis à l'aide d'un instrument spécifique, ou au clavier, dans le cas des spectres établis par compilation externe. Les spectres de masse ainsi obtenus peuvent être mis en mémoire en BASIC Finnigan sur bande magnétique ce qui permet d'autres opérations BASIC, ou sur disques magnétiques dans l'ordinateur, ce qui permet la manipulation ordinaire des spectres de masse par le système d'exploitation.

## INTRODUCTION

The Gas Chromatograph/Mass Spectrometer/Data System (GC/MS/DS) can be a very powerful analytical tool in the rapid, positive identification of unknown compounds in complex mixtures. Liquid sample mixtures whether from laboratory reactions or extracted from vegetation, soil, water or air can be injected into the GC for separation and analysed quickly by the MS. Although it is possible for an experienced mass spectroscopist to examine a specific mass spectrum and deduce the structure of an unknown compound in the sample, time constraints require that more rapid identification be carried out. The key to rapid accurate identification lies in the use of an integrated data system containing a library search algorithm and an extensive collection of standard mass spectra or edited representations. In use, the search algorithm package compares a representation of the mass spectrum of the unknown compound with mass spectra contained in the library and lists, in descending order of "goodness of fit", several retrieved compounds whose mass spectra most closely resemble that of the unknown. Obviously, the greater the number of different types of compounds represented in the library, the greater is the accuracy of the identification of the unknown or, at least, the family of compounds to which the unknown belongs. The commercial libraries contain limited numbers of spectra of common chemicals but many permit the addition of new entries. Consequently, after acquisition of a GC/MS/DS system incorporating a search algorithm, one of the initial requirements in the preparation of the system for use as a rapid analytical identification tool for specific classes of compounds is to have available related mass spectra, either by recording the spectra on the specific GC/MS or by manually entering them from other sources (reports,compilations etc.).

In some library search programs, the mass spectrum is abbreviated or edited before it can either be compared to the library entries or be added as a library entry. In these systems, then, although a given library entry can be subsequently recalled and listed, a significant amount of information has been lost during the editing process. Occasions may arise in which ready display or output of the complete mass spectrum of the library compound is desirable to permit critical assessments to be made as to the accuracy of a given identification. Furthermore, new searching programs are becoming available which incorporate highly sophisticated searching algorithms requiring more complete mass spectra to be stored as library entries. Introduction of such a system would normally require re-entry of large numbers of complete mass spectra for editing according to the specific code of the searching algorithm.

A separate and compact storage of relevant mass spectra is desirable to permit rapid incorporation into new searching systems and specific recall and display of complete mass spectra. In order that these requirements be met, several BASIC (1) programs have been developed to permit files of mass spectra, whether from a Finnigan GC/MS/DS or from outside sources, to be entered and stored for later display and/or incorporation into new library search algorithms as they become available. The programs, written in Finnigan BASIC, can be used on any Finnigan GC/MS employing a 6115 Data system.

## PROGRAM DESCRIPTIONS AND OPERATIONS

### PROGRAM SPECFL

This program is designed to build a compact computer file of mass spectra from either the GC/MS/DS or from outside compilations. The program consists of a main body (statements 2-240, 9995-9999) which permits the user to select various operations, a number of subprograms (statements 1000-6220) which can be called upon by the main program to perform the individual operations and a DATA area (statements 7001-9994) in which titles of the individual entries are stored. Some of the subprograms also present the user with further options or request additional information during execution.

Basically, an entry in the file consists of two parts; the title and the mass spectral listing. The title contains the molecular weight, the base peak, a formula code, a name of 36 letters and four spaces for a code or abbreviated name. In the example below, the molecular weight is 198; the base peak, 119; number of carbons, 04; hydrogens, 12; bromine, 1; chlorine, 0; fluorine, 0; iodine, 0; nitrogen, 2; oxygen, 0; phosphorous, 1; sulfur, 0; and other, 0.

198 119 .4121...2.1..BIS(DIMETHYLAMINO) BROMOPHOSPHINE

The title is stored as an integral part of the program in the form of a DATA statement beginning with entry #1 at statement 7001. By storing the titles as part of the program, storage of mass spectral data is confined to one additional data tape. Furthermore, by storing the title information in this manner, the status search of the files (entry numbers of filled entries for the next addition, or for compounds of a selected molecular weight and/or base peak) is rapidly executed without further tape or disc manipulation. A deletion is made by simply rewriting the particular DATA statement as one having a blank field. Essentially, then, a title addition or deletion is the rewriting of a statement of the program during execution. The end of the DATA section (statement 9994) is indicated by an entry whose molecular weight is "000".

The mass spectral listing is stored on magnetic tape in Finnigan BASIC DATA format as a one-dimensional array of ion abundances of m/e of 0 to 1000. The absolute abundances of m/e of 0-11 and 1000 are reserved for storage of other pertinent information, e.g. m/e of 0 is the entry number, m/e of 1 is the molecular weight, m/e of 2 is the base peak, m/e of 3 is an indicator as to whether the spectrum is electron impact (EIMS) or chemical ionization (CIMS) and m/e of 4 is the highest non-zero m/e. These values are included to permit subsequent sorting or searching by other BASIC programs should the need arise. Other information could readily be added in m/e (5) - m/e (11) and m/e (1000) by slight modification to the program if desired.

A typical operation of the program such as the addition of a mass spectrum involves the transfer of a selected number of consecutive preceeding existing mass spectra from tape to disc (usually only the preceeding mass spectrum to minimize tape-to-disc transfers), the spectrum entry from computer memory (if the spectrum has been recorded on the GC/MS) or typewriter (from outside compilation), and the transfer of succeeding mass spectra from tape to disc if the addition is an insertion into a file rather than an addition to the end of one. The spectra stored on disc are not in BASIC but

the language of the operating system (designated herein as FOS) and, as such, can be manipulated, plotted out, listed, etc. in the same manner as an internally generated file. A single disc file can store up to 1000 mass spectra or scans. During the file development phase, blocks of 100 or less spectra are constructed due to a 100-file-name limitation on a BASIC tape. Spectra added to the end of a disc file during program execution may be easily added to existing spectra on the BASIC tape (up to 100 entries) by use of DTRDFN. Successive disc files of 100 can be united into larger disc collections of up to 1000 entries by use of DISCFL. Once a file of 1000 spectra (or less) has been built up, the file may be more compactly stored on tape in FOS permitting a significantly more rapid tape-to-disc transfer than is possible in Finnigan BASIC. The program is capable of holding nearly 3000 titles (subject to overall computer memory availability) and thus can be used in conjunction with development of three successive disc files before another separate copy of the program is necessary. A brief description of the program operation and required input follows; a detailed flow chart, variable index and glossary and program listing are given in Appendix I. The program can be broken into several subsections:

MAIN BODY (Statements 2-240, 9995-9999)

The object of the main body is to present the various options to the user and to call upon the appropriate subprograms to execute the options as selected. The following are the main steps for the use of the main body:

1. The program is transferred from BASIC program tape to memory and RUN is entered.

2. During execution, the program will stop at statement 14 to permit alteration of statements 15-79. Statement 15 is the name of the FOS disc file (6 characters maximum) into which the spectra are to be read and statements 16-79 contain names of each mass spectrum as it is stored on BASIC data tape (in this case, the names are numbers corresponding in order to the titles and to the entries for the absolute abundance of m/e of 0 in each spectrum to facilitate rapid identification and cross-referencing).

3. The user indicates which BASIC data tape is being modified i.e. spectra 1-100, 100-200, etc.

4. The user indicates the entry number of the first mass spectrum to be transferred from BASIC data tape to FOS disc (usually only one or two before entry to be added).

5. The user indicates if an upper limit on the number of spectra to be transferred is necessary and, if so, the number of the last entry to be transferred from tape to disc. This is necessary when alterations (deletions or additions to previously-deleted entries) are made to otherwise-filled tapes. Without this limitation, the program would attempt to transfer spectra with entry numbers greater than those contained on the specific tape. It should be noted that in the case of deletions or readditions to a data tape all spectra must also be transferred and the

tape erased to facilitate consecutive repacking of the tape using DTRDFN.

6. The first option is a listing of the file status based on a search of all the title statements. The last filled location and the first blank location are identified by entry number (the entire file is tight-packed so that any new entry is located in the first available blank space be it the result of a deleted entry or alternatively at the end of the filled entries). This operation is carried out internally for most other options but output and other sub-options in subprogram 1 (SPI) are not provided if the option has not been specifically selected by the user.

7. The second option is the addition of mass spectra with associated titles. If the entry is made at the end of a file, i.e. there are no empty spaces due to deletions, subsequent consecutive entries are permitted in subprogram 2 (SP2) without re-execution of the entire program. If this option is chosen, the following option is not available.

8. The third option is the deletion by subprogram 3 (SP3) of a single mass spectrum with its associated title from anywhere within the filled locations of the 100-entry mass spectral tape file currently under development.

9. The fourth option is the output of spectral files. Titles and/or mass spectral listings of entries are printed out by subprogram 4 (SP4). Selections for mass spectral listings are limited to the 100-entry tape file currently under development but any title can be printed from the entire collection.

10. The program is rewritten on BASIC program tape under a new name to save any title changes. A single data file remains on disc in FOS containing the transferred preceeding spectra, the added (or, in the case of a deletion, a zeroed) spectrum and all filled succeeding entries of the file under development subject to initially specified limitations. Selected consecutive spectra of a FOS file containing added spectra can be added to the end of the BASIC tape under development by using DTRDFN.

SUBPROGRAM 1 (SP1, 1000-1540)

This option presents the current status of the entire file by examining the titles in the DATA statements. The main features are as follows:

1. The program calls upon subprogram 5 (SP5) to determine which title spaces are empty and where the last filled entry has been made. The results of the search are printed out.

2. The user may further call for a list of the entry numbers of those compounds with a specific molecular weight (MW) and/or mass spectral base peak (BP). The choice of MW or BP is entered as a 3-digit number (including a leading 0 if the number is less than 100) contained between quotes, e.g. "042".

3. Additional choices for other MW or BP searches can be made after which control is returned to the main body of the program.

SUBPROGRAM 2 (SP2, Statements 2000-2590)

This option adds mass spectra to the file. The main features follow:

1. If the previous option has not been exercised, SP2 calls upon SP5 to determine which title spaces are filled and which are empty. The entry number for the current addition, internally-determined for maintenance of tight-packed file structure, is then printed out.

2. The user indicates whether the new spectrum is resident in FOS memory or is to be entered by typewriter.

3. Subprogram 7 (SP7) is called upon to transfer the selected preceeding spectra up to the designated entry number from tape to disc. The value of m/e of zero for the mass spectrum to be added is set equal to the entry number.

4. The user indicates whether the new entry is an electron impact or chemical ionization mass spectrum and this is stored as the abundance of m/e of 3.

5. The user provides the molecular weight of the compound which is stored as the abundance of m/e of 1.

6. The spectrum is entered. An entry from FOS memory is automatic while manual introduction is accomplished by entering pairs of numbers in which the first is the m/e while the second is the corresponding abundance, relative or absolute. Errors in input can be corrected by simply reentering the corrected version and rezeroing the abundance of an incorrectly-entered m/e. The end of input is signalled by entering 9999 for m/e.

7. Subprogram 6 (SP6) is called for normalization of the mass spectrum to the internally-determined base peak. The m/e of the base peak and largest non-zero m/e are printed out and automatically entered as the abundance of m/e at 2 and 4 for future sorting or collating programs. The spectrum is then added to the disc file.

8. If this addition is not being made at the end of a file but as a replacement for an earlier deletion, the corresponding spectrum (currently stored as a series of zeros) is read from the tape to maintain proper spectrum sequencing. SP7 is then recalled to transfer the remaining spectra (subject to initially imposed limits) to the disc and the disc file is closed. If, however, the addition is made to the end of the BASIC tape files, additional successive mass spectra may be manually added at the user's discretion.

9. The corresponding titles of the mass spectra are entered by adding the appropriate DATA statements (#1 entry corresponds to program statement #7001).

10. Three specified constants must be reentered following completion of title introduction to recommence program execution by returning control to the main body of the program.

SUBPROGRAM 3(SP3, Statements 3000-3300)

This option permits deletion of one mass spectrum from the tape file under development. It has been restricted to a single deletion since large scale deletions are unlikely to be necessary. Changes to the program could be readily introduced to remove this limitation if required. The following points summarize the operation of SP3:

1. The entry number of the mass spectrum to be deleted is introduced.

2. SP5 is called to establish the location of the last filled space in the file for transfer purposes.

3. SP7 is called to transfer the selected preceeding mass spectra up to the one designated for deletion from tape to disc.

4. The designated spectrum is read from the tape to maintain proper tape sequence, all m/e abundances are zeroed and the zeroed mass spectrum recorded on disc.

5. SP7 is called to complete transfer of the remaining mass spectra from tape to disc and the disc file is closed.

6. The appropriate title is rewritten as a blank DATA statement (#1 entry corresponds to program statement #7001).

7. Three specified constants must be reentered after the title change to resume program execution by returning control program main body.

SUBPROGRAM 4(SP4, Statements 4000-4340)

This option provides a listing of one or more consecutive titles and/or mass spectra. If no mass spectra are desired, no transfer of data from tape to disc occurs. If mass spectra are required, transfer is carried out unless it has already occurred due to selection of either options SP2 or SP3. The output of a mass spectral listing is possible only if it is included in the consecutive collection of spectra requested at the beginning of the program main body for transfer from tape to disc and the corresponding BASIC data tape is in use. The main points of SP4 are as follows:

1. The selection of consecutive entry numbers for output is made by introducing the first and last number of the range. If only one is required, the same number is entered for both limits. A choice of whether the output will be titles and/or mass spectra is also indicated.

2. If mass spectra are required, transfer from tape to disc is carried out unless either SP2 or SP3 has already operated.

3. If titles are required, DATA statements up to but not including the first member of the designated range are read and disregarded to maintain proper sequence and numbering.

4. For each of the entries in the indicated range, the title is read and printed (if required) and the mass spectrum is read from disc and listed (if required).

5. Control is transferred back to the main body of the program.

SUBPROGRAM 5(SP5, Statements 5000-5210)

This subprogram searches through the titles and compares each entry with two defined DATA statements: the first comparison to determine if the end of the list of titles has been reached; the second to determine if the title is blank signalling a previously-deleted file. Provision has also been made for a warning if there are no remaining blank files on the tape due to the BASIC computer limit of 100 file names on a single tape. On completion of the search, control is transferred back to the main body.

SUBPROGRAM 6(SP6, Statements 6000-6080)

In this subprogram the base peak and highest non-zero m/e are determined, stored as the absolute abundances of m/e of 2 and 4 and printed out. The subprogram finishes by normalizing the spectrum and multiplying the resultant relative abundances by 100 to permit adequate subsequent oscilloscope display of minor peaks in the FOS.

SUBPROGRAM 7(SP7, Statements 6100-6220)

This subprogram transfers mass spectra from BASIC data tape to FOS disc. The first spectrum or scan of a disc file is written as a zeroed mass spectrum to maintain the correct numbering correspondence with the titles since the FOS has a zero scan included for internal manipulations of disc files. Other important points to be noted about SP7 follow:

1. The FOS disc file will automatically be titled "File of Individual Spectra". Other titles are possible by alternation of statement 6105.

2. Mass spectral entries from C1 to C2 are read from tape to disc.

3. The disc file is left unclosed so that subsequent files may be added by the calling program. Control then is passed back to the calling program.

ALTERNATE USE OF SPECFL

After a larger disc file of up to 1000 spectra has been developed using DISCFL and several 100-spectra disc files, access to and output of spectra from the disc file (separate from the manipulations possible in FOS) can be made possible by modifying SPECFL. The program then becomes one which will output file status and titles from the DATA statements and/or mass spectra from the disc file identified in statement 15.

```
80 LET S = 1
82 LET Q3 = number of spectra on file
83 GO TO 94
102 GO TO 190
4150 DREAD #1, I, N
and statements 81, 4130 and 5016 are deleted.
```

A duplicate copy of the program with the following change accesses the second disc file of 1000 spectra if the appropriate disc file name is entered in statement 15.

```
4150 DREAD #1, I-1000, N
```

and so on for each successive disc file.

PROGRAM DTRDFN

On the completion of a SPECFL execution, a data file remains on disc in FOS containing a number of spectra. The contents of this single file in FOS must be transferred back to tape in the form of individual data files in BASIC, one for each spectrum, for subsequent file additions or deletions. DTRDFN, of which a listing, flow chart, variable index and glossary appear in Appendix II, carries out the transfer from disc to tape. As indicated

earlier, if a deletion or a spectral replacement in a previously-deleted space has been carried out, all spectra must be deleted from the BASIC data tape before a subsequent disc-to-tape transfer of the entire tape file of spectra is attempted to avoid error messages due to duplicate file names and to maintain proper sequencing of spectra. Additions to the end of the tape file are made without alteration of other spectra on the tape. As in SPECFL, statement 15 in DTRDFN gives the name of the disc file while 16-79 contain names to be assigned to the individual mass spectra as they are written on tape. With appropriate changes to statement 16-79, the program can be used to fill several tapes with spectra numbered consecutively from 1 onward. The major features of this program follow:

1. An initial STOP statement allows the user to rewrite any of statements 15-79 to accommodate any FOS disc file and to assign any BASIC tape file name desired.

2. The entry numbers of the spectra to be transferred are entered. This is followed by the entry number of the first spectrum on the disc file to maintain correspondence of file numbering on the tape with spectra being transferred.

3. The program indicates when the operation is complete.

PROGRAM DISCFL

For manipulation by the operating system, rapidity of disc-tape data transfer and compact tape storage, the final completed spectral file is written in the language of the operating system (disc format). The program DISCFL is designed to transfer a number of smaller disc files of 100 spectra or less directly into a single composite disc file of up to 1000 spectra. A listing, flow chart, variable index and glossary of the program is given in Appendix III.

The main points for use of DISCFL follow:

1. The file name of the composite disc file is written in statement 15 and the names of the source disc files are included in statements 16-19 in the order in which the spectra are stored i.e. 1-100, 101-200 etc.

2. An initial blank spectrum is entered by the program into scan #0 of the composite disc file (see discussion in SP7 in SPECFL).

3. The number of disc files to be merged is entered. In turn, the number of spectra to be read from each disc file into the composite file is entered recalling that each new disc file starts at spectra #1 even if spectrum #101 is stored there.

4. The program indicates when the task is completed.

PROGRAM TRANTD

This short program substitutes in place of SPECFL when only transfer of mass spectral files from BASIC tape to FOS disc files is desired with no requirement for deletions, additions, output or file status reports. A listing, flow chart, variable index and glossary of the program are given in Appendix IV. The main points follow:

1. As in the other programs, the disc file name is written in statement 15 with tape file names, in order, in statements 16-99.

2. The initial spectrum written on disc is a blank as in previous programs.

3. The entry numbers of the first and last mass spectra to be transferred are entered.

4. The program indicates when the task is completed.

## REFERENCES

1. Finnigan BASIC Reference Manual, REV. I, Finnigan Corporation, 1977.

## APPENDIX I

### VARIABLE GLOSSARY - SPECFL

A(I) - A one-dimensional array for storage of entry numbers of compounds having a specific molecular weight.

A$(I) - A one-dimensional array for temporary storage of mass spectral title information.

B(I) - A one-dimensional array for storage of compounds having a specific mass spectral base peak.

B$(I) - A one-dimensional array used in searching for empty mass spectral title files and for storage of selected molecular weights and/or mass spectral base peaks during searches of mass spectral title files.

D$(I) - A one-dimensional array for storage of overall title information of the disc file containing mass spectra.

E$(I) - A three-character one-dimensional array used to indicate the end of DATA statements.

M(I) - A one-dimensional array containing a mass spectrum recorded by the FOS. A spectrum must be stored in FOS memory and intention to input a mass spectrum from FOS be specified prior to loading the BASIC program.

N(I) - A one-dimensional array containing ion abundance for $^{m}/e$ of 12-999 of a mass spectrum and other special information in N(0) - N(11) and N(1000).

A1 - Selection indicator for listing of status of title files based on: 1 - desired, 2 - not desired.

A2 - Selection indicator for addition of mass spectra to file based on: 1 - desired, 2 - not desired.

A3 - Selection indicator for deletion of a mass spectrum from file based on: 1 - desired, 2 - not desired.

VARIABLE GLOSSARY - SPECFL

A4 - Selection indicator for output of mass spectral titles and/or data based on: 1 - desired, 2 - not desired.

A5 - Selection indicator for placing an upper limit of number of tape files transferred based on: 1 - limit, 2 - no limit.

A6 - Selection indicator for entry number of last spectrum to be transferred from loaded tape to disc.

A8 - Selection indicator for output of titles of compounds with a specific molecular weight based on: 1 - desired, 2 - not desired.

A9 - Selection indicator for output of titles of compounds with a specific base peak based on: 1 - desired, 2 - not desired.

B - Variable used for storage of entry number of first empty mass spectral title and data space in file.

B1 - Variable used for storage of number of compounds with a specific molecular weight.

B2 - Variable used for storage of number of compounds with a specific mass spectral base peak.

B3 - Selection indicator for entry number of mass spectrum to be deleted from the file.

B5 - Selection indicator for initial entry number of range of entries of mass spectral titles and/or data to be printed out.

B6 - Selection indicator for output of mass spectral titles based on: 1 - desired, 2 - not desired.

B7 - Selection indicator for output of mass spectral data based on: 1 - desired, 2 - not desired.

B8 - Selection indicator for final entry number of range of entries of mass spectral titles and/or data to be printed out.

C - Variable used for storage of entry number of last-filled mass spectral title and data space in file.

C1 - Variable used for identification of initial data file in a tape-to-disc transfer.

C2 - Variable used for identification of final data file in a tape-to-disc transfer.

D1 - Selection indicator for source of mass spectrum to be added to file based on: 1 - FOS memory, 2 - manual entry.

D3 - Selection indicator for addition of consecutive mass spectra to the file based on: 1 - desired, 2 - not desired.

D4 - Selection indicator for additional output of mass spectral titles/ data based on: 1 - desired, 2 - not desired.

G - Variable used for storage of entry number of first empty data space available on file for addition of a new mass spectrum.

C9 - Variable used to modify tape file number for entry of mass spectrum to the disc file.

H - Variable used for storage of abundance of mass spectral base peak.

K - Selection indicator for entry of specific m/e.

L - Selection indicator for entry of a specific absolute abundance.

Q1 - Variable used to indicate which data tape is currently under development.

Q2 - Variable used for storage of entry number of first mass spectrum to be transferred from tape to disc.

Q3 - Variable used for storage of maximum entry number of last mass spectrum on tape.

S - Variable used as an indicator of transfer of mass spectral data from tape-to-disc based on: 0 - no transfer, 1 - transfer has already occurred.

T - Variable used for storage or assignment of tape file names.

X - Selection indicator for printout of titles of compounds with a specific molecular weight or specific mass spectral base peak based on, <3 - output desired for at least one list, >3 - neither list required.

Z - Selection indicator for additional output of entry numbers for compounds with a specific molecular weight and/or base peak based on: 1 - more required, 2 - no further output required.

VARIABLE INDEX - SPECFL

| Variable | Statement No. |
|---|---|
| A(I) | 10,1098,1320,1440 |
| A$(I) | 10,1270,1290,1340,4080,4103,4110,4115,5025,5030,5050, 5170,5175,5180 |
| B(I) | 10,1098,1370,1500 |
| B$(I) | 10,1130,1210,1290,1340,1410,1470,5000,5050,5180 |
| D$(I) | 10,2382,3245,6105,6106,6130 |
| E$(I) | 10,5010,5030,5175 |
| M(I) | 2060,2230 |
| N(I) | 10,2160,2170,2183,2185,2200,2210,2230,2290,2382,2393, 3231,3241,3242,3244,3245,4150,4154,4155,4163,4185,4190, 4191,6007,6009,6010,6015,6020,6030,6035,6050,6060,6102, 6103,6106,6127,6130 |
| A1 | 96,98,2000 |
| A2 | 104,110 |
| A3 | 150,160 |
| A4 | 200,210 |
| A5 | 87,89,2500,3262,4056 |
| A6 | 92,2510,3264,4057 |
| A8 | 1050,1095,1100,1280,1400 |
| A9 | 1080,1095,1180,1330,1460 |
| B | 1006,1010,2010,2025,5035,5065,5140,5160 |
| B1 | 1170,1300,1320,1410,1415,1430 |
| B2 | 1250,1350,1370,1470,1475,1490 |
| B3 | 3010,3075,3220,3250 |
| B5 | 4010,4065,4070,4101 |
| B6 | 4030,4062,4102 |
| B7 | 4050,4051,4120 |
| B8 | 4010,4101 |
| C | 1007,1020,1260,2387,2410,2490,2586,2588,3260,3293,3295, 4055,5040,5066,5150,5190 |
| C1 | 2020,2480,3071,3250,4054,6100,6109,6110 |
| C2 | 2025,2490,2510,3075,3260,3264,4055,4057,6109,6110 |
| D1 | 2110,2215 |
| D3 | 2440,2450 |
| D4 | 4220,4230 |

VARIABLE INDEX - SPECFL

| Variable | Statement No. |
|---|---|
| G | 2010,2050,2185,2460,2480 |
| G9 | 4130,4150 |
| H | 6000,6010,6015,6060 |
| K | 2285,2287,2290 |
| L | 2285,2290 |
| Q1 | 82,2586,2588,3293,3295,5016 |
| Q2 | 84,2020,2586,2588,3071,3293,3295,4054,4130,6100 |
| Q3 | 1006,1007,5016,5020,5065,5066,5080,5100,5160 |
| S | 80,2130,2385,2589,3297,4052,4060 |
| T | 2386,2387,2393,3220,3231,6111,6127 |
| X | 1095,1096 |
| Z | 1516,1517 |

## APPENDIX I

## PROGRAM LISTING - SPECFL

```
5    REM THIS PROGRAM CAN ADD ENTRIES TO OR LIST OR DELETE ENTRIES FROM
6    REM A LIBRARY OF COMPLETE MASS SPECTRA
10   DIM N(1ØØ1),A(1ØØ),B(1ØØ),A$(6Ø),B$(7),D$(48),E$(3)
11   PRINT"DATA FILES CONTAINING SPECTRA MUST EXIST ON TAPE UNDER FILE"
12   PRINT"NAME AS 1,2,3..;THESE FILE NAMES START AT STATEMENT 16;DISC"
13   PRINT"FILE NAME IS AT STATEMENT 15**TO START PROGRAM-'GO TO 15'"
14   STOP
15   FILES EXTRØ5
16   FILES 1,2,3,4,5,6,7,8,9,1Ø,11,12,13,14,15,16,17,18,19,2Ø,21,22,23,24
17   FILES 25,26,27,28,29,3Ø,31,32,33,34,35,36,37,38,39,4Ø,41,42,43,44,45
18   FILES 46,47,48,49,5Ø,51,52,53,54,55,56,57,58,59,6Ø,61,62,63,64,65,66
19   FILES 67,68,69,7Ø,71,72,73,74,75,76,77,78,79,8Ø,81,82,83,84,85,86,87
20   FILES 88,89,9Ø,91,92,93,94,95,96,97,98,99,1ØØ,1Ø1,1Ø2,1Ø3,1Ø4,1Ø5,1Ø6
80   LET S=Ø
81   PRINT"WHICH TAPE IS LOADED? 1=1-1ØØ;2=1Ø1-2ØØ;ETC.";
82   INPUT Q1
83   PRINT"ENTER NUMBER OF FIRST SPECTRUM TO BE TRANSFERRED";
84   INPUT Q2
85   PRINT"DO YOU WISH AN UPPER LIMIT ON FILE TRANSFER?1=YES;2=NO";
87   INPUT A5
89   IF A5 > 1 THEN 94
90   PRINT"ENTER NUMBER OF LAST SPECTRUM TO BE TRANSFERRED";
92   INPUT A6
94   PRINT"DO YOU WISH TO LIST STATUS OF SPECTRAL FILES? 1=YES;2=NO";
96   INPUT A1
98   IF A1 > 1 THEN 1Ø2
100  GO SUB 1ØØØ
102  PRINT"DO YOU WISH TO ADD TO SPECTRAL FILES? 1=YES;2=NO";
104  INPUT A2
110  IF A2 > 1 THEN 14Ø
125  GO SUB 2ØØØ
140  PRINT"DO YOU WISH TO DELETE SPECTRAL FILES? 1=YES;2=NO";
150  INPUT A3
160  IF A3 > 1 THEN 190
165  GO SUB 3ØØØ
190  PRINT"DO YOU WISH TO OUTPUT SPECTRAL FILES? 1=YES;2=NO";
200  INPUT A4
210  IF A4 > 1 THEN 240
230  GO SUB 4ØØØ
240  GO TO 9995
1000 GO SUB 5ØØØ
1005 PRINT
1006 IF B> Q3 THEN 1030
1007 IF C=Q3 THEN 1030
1010 PRINT"THE FIRST EMPTY DATA NAME SPACE IS NUMBER ";B;" AND THE LAST"
1020 PRINT"FILLED ONE IS NUMBER ";C
1030 PRINT"DO YOU WISH TO OUTPUT A LIST OF COMPOUNDS WITH A SPECIFIC"
1040 PRINT"MOLECULAR WEIGHT? 1=YES;2=NO";
1050 INPUT A8
1060 PRINT"DO YOU WISH TO OUTPUT A LIST OF COMPOUNDS WITH A SPECIFIC"
1070 PRINT"BASE PEAK? 1=YES;2=NO";
1080 INPUT A9
1095 LET X=A8+A9
1096 IF X > 3 THEN 1540
1097 FOR I=1 TO 1ØØ STEP 1
1098 LET A(I)=B(I)=Ø
1099 NEXT I
1100 IF A8 > 1 THEN 1180
1110 PRINT"INPUT A 3-DIGIT (INCLUDING A LEADING Ø IF APPLICABLE) MW IN"
1120 PRINT"QUOTES AS 'XXX'";
1130 INPUT B$(Ø,2)
1170 LET B1=Ø
1180 IF A9 > 1 THEN 1260
1190 PRINT"INPUT A 3-DIGIT (INCLUDING A LEADING Ø IF APPLICABLE) BP IN"
1200 PRINT"QUOTES AS 'XXX'";
```

## APPENDIX I

## PROGRAM LISTING - SPECFL

```
1210 INPUT B$(4,6)
1250 LET B2=Ø
1260 FOR I=1 TO C STEP 1
1270 READ A$
1280 IF A8 > 1 THEN 133Ø
1290 IF A$(Ø,2)<> B$(Ø,2) THEN 1330
1300 LET B1=B1+1
1320 LET A(B1)=1
1330 IF A9 > 1 THEN 1380
1340 IF A$(4,6)<>B$(4,6) THEN 138Ø
1350 LET B2=B2+1
1370 LET B(B2)=I
1380 NEXT I
1390 RESTORE
1400 IF A8 >1 THEN 1460
1405 PRINT
1410 PRINT"THERE ARE ";B1;" ENTRIES WITH MOLECULAR WEIGHT OF ";B$(Ø,2)
1415 IF B1=Ø THEN 1460
1420 PRINT"AND THESE OCCUR AT THE FOLLOWING ENTRY NUMBERS:"
1430 FOR I=1 TO B1 STEP 7
1440 PRINT A(I);A(I+1);A(I+2);A(I+3);A(I+4);A(I+5);A(I+6)
1450 NEXT I
1460 IF A9 >1 THEN 1515
1465 PRINT
1470 PRINT"THERE ARE ";B2;" ENTRIES WITH BASE PEAK AT ";B$(4,6)
1475 IF B2=Ø THEN 1515
1480 PRINT"AND THESE OCCUR AT THE FOLLOWING ENTRY NUMBERS:"
1490 FOR I=1 TO B2 STEP 7
1500 PRINT B(I); B(I+1);B(I+2);B(I+3);B(I+4);B(I+5);B(I+6)
1510 NEXT I
1515 PRINT"DO YOU WISH MORE LISTINGS? 1=YES;2=NO";
1516 INPUT Z
1517 IF Z=1 THEN 1Ø3Ø
1520 PRINT
1540 RETURN
2000 IF A1=1 THEN 2Ø1Ø
2005 GO SUB 5ØØØ
2010 LET G=B
2020 LET C1=Q2
2025 LET C2=B-1
2050 PRINT"THIS ENTRY WILL BE MADE AT NUMBER";G;"PROCEED AS FOLLOWS:"
2060 PRINT"FIRST' THE SPECTRUM IS ENTERED; 1=IN M(ABS);2=MANUALLY BY 7ØØ";
2110 INPUT D1
2130 IF S > Ø THEN 2150
2140 GO SUB 6100
2150 FOR J=Ø TO 99Ø STEP 1Ø
2160 LET N(J)=N(J+1)=N(J+2)=N(J+3)=N(J+4)=N(J+5)=Ø
2170 LET N(J+6)=N(J+7)=N(J+8)=N(J+9)=Ø
2180 NEXT J
2183 LET N(1ØØØ)=Ø
2185 LET N(Ø)=G
2190 PRINT"IS THIS SPECTRUM EI(=Ø) OR CI(=1)";
2200 INPUT N(3)
2205 PRINT"INPUT THE MOLECULAR WT. OF THIS COMPOUND";
2210 INPUT N(1)
2215 IF D1=2 THEN 2255
2220 FOR J=12 TO 999 STEP 1
2230 LET N(J)=M(J)
2240 NEXT J
2250 GO TO 2310
2255 PRINT
2260 PRINT"INPUT M/E AND INTENSITY FOR EACH ENTRY;ON COMPLETION,ENTER"
2261 PRINT"9999 FOR M/E;CORRECTIONS ARE MADE BY REENTERING CORRECTED"
2262 PRINT"VERSION AS WELL AS A ZERO INTENSITY FOR MISTAKEN M/E IF"
2263 PRINT"ERROR EXISTED IN THE M/E PORTION OF ENTRY(OTHER THAN M/E OF"
```

## APPENDIX I

### PROGRAM LISTING - SPECFL

```
2264 PRINT"Ø-4 WHICH ARE ENT#,MW,BP,EI/C1 AND MOL.ION.M/E INDICATORS"
2285 INPUT K,L
2287 IF K=9999 THEN 2310
2290 LET N(K)=L
2300 GO TO 2285
2310 GO SUB 6ØØØ
2382 DWRITE#1,D$,N
2385 LET S=1
2386 LET T=T+1
2387 IF T > (C+1) THEN 2410
2392 FOR J=Ø TO 1ØØØ STEP 1
2393 CREAD #T,N(J)
2395 NEXT J
2397 GO TO 2480
2410 LET C=C+1
2415 PRINT
2420 PRINT"THERE ARE SUCCESSIVE EMPTY FILES;DO YOU WISH TO ADD MORE"
2430 PRINT"FILES AT THIS TIME? 1=YES;2=NO";
2440 INPUT D3
2450 IF D3 > 1 THEN 2575
2460 LET G=G+1
2470 GO TO 2Ø5Ø
2480 LET C1=G+1
2490 LET C2=C
2500 IF A5 > 1 THEN 256Ø
2510 LET C2=A6
2560 GO SUB 61ØØ
2575 EOF #1
2580 PRINT
2581 PRINT"SECOND,THE TITLES OR ALPHATEXT ARE REQUIRED;ENTER THE DATA"
2582 PRINT"IN THE FOLLOWING MANNER..XXXX DATA 'TITLE'..WHERE TITLE IS"
2583 PRINT"MOL.WT.(3),X,BASE PK.(3),X,C(2),H(2),BR(1),CL(1),F(1),I(1),"
2584 PRINT"N(1),O(1),P(1),S(1),ME(1),AND 32-67 FOR NAME ETC. AND 68-71"
2585 PRINT"FOR CODE DESIGNATION ETC."
2586 PRINT"THEN TYPE GO TO 2588 FOLLOWING BY INPUT OF ";Q1;C;Q2
2587 STOP
2588 INPUT Q1,C,Q2
2589 LET S=1
2590 GO TO 19Ø
3000 PRINT"INPUT THE ENTRY NUMBER OF FILE WHICH IS TO BE DELETED";
3010 INPUT B3
3070 GO SUB 5ØØØ
3071 LET C1=Q2
3075 LET C2=B3-1
3200 GO SUB 61ØØ
3220 LET T=B3+1
3230 FOR J=Ø TO 1ØØØ STEP 1
3231 CREAD #T,N(J)
3232 NEXT J
3240 FOR J=Ø TO 99Ø STEP 1Ø
3241 LET N(J)=N(J+1)=N(J+2)=N(J+3)=N(J+4)=N(J+5)=Ø
3242 LET N(J+6)=N(J+7)=N(J+8)=N(J+9)=Ø
3243 NEXT J
3244 LET N(1ØØØ)=Ø
3245 DWRITE #1,D$,N
3250 LET C1=B3+1
3260 LET C2=C
3262 IF A5 > 1 THEN 3270
3264 LET C2=A6
3270 GO SUB 61ØØ
3280 EOF #1
3291 PRINT"SECOND, THE ALPHATEXT IS DELETED BY TYPING IN THE FOLLOWING:"
3292 PRINT"XXXX DATA'6Ø BLANKS...'AND THEN-GO TO 3295-FOLLOWED BY"
3293 PRINT"INPUT OF THE FOLLOWING NUMBERS";Q1;C;Q2
3294 STOP
```

## APPENDIX I

## PROGRAM LISTING - SPECFL

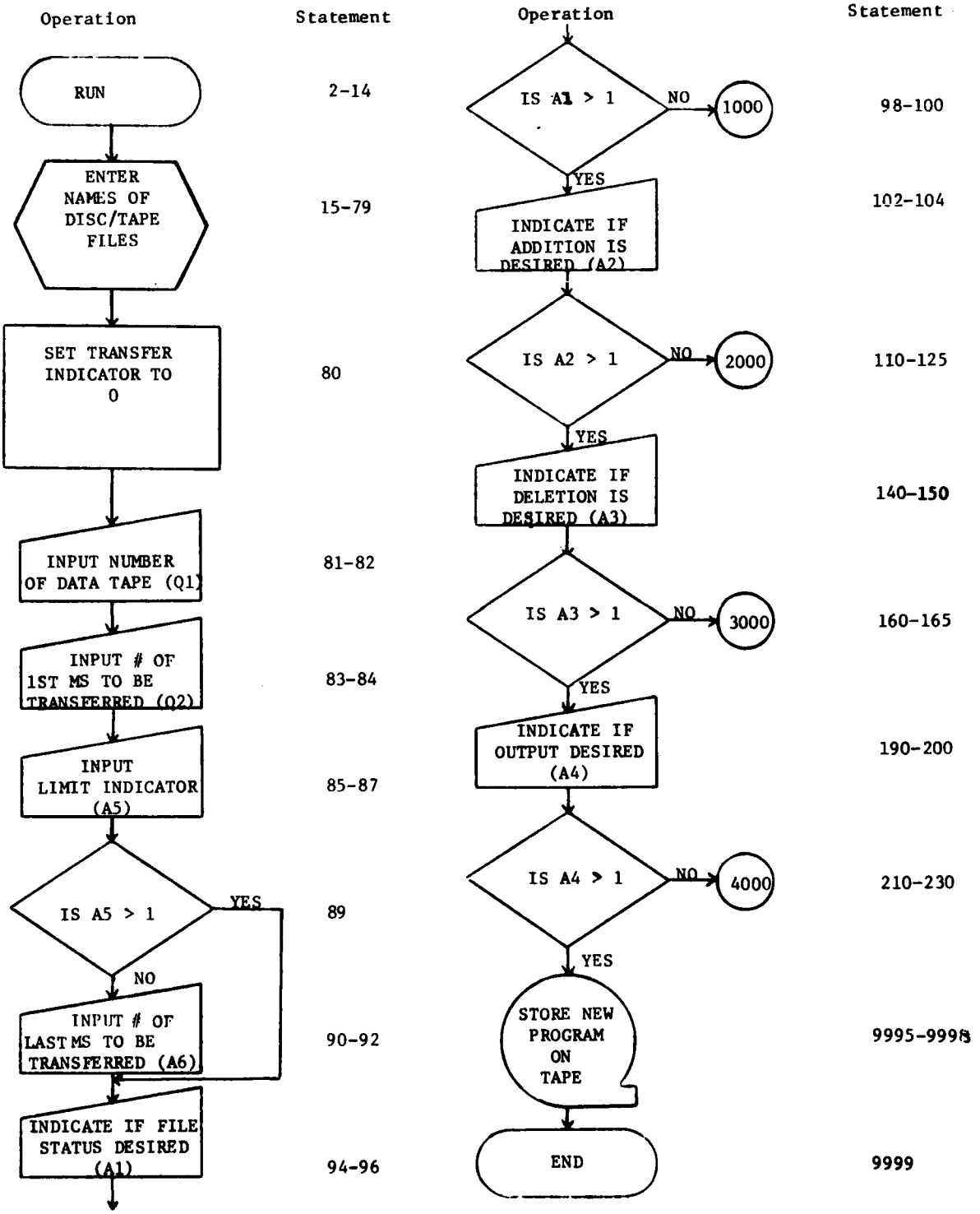
```
3295 INPUT Q1,C,Q2
3297 LET S=1
3300 GO TO 190
4000 PRINT"INPUT SPECTRUM NUMBERS DESIRED (2 NUMBERS TO DEFINE RANGE)";
4010 INPUT B5,B8
4020 PRINT"DO YOU WISH ALPHA TEXT? 1=YES;2=NO";
4030 INPUT B6
4040 PRINT"DO YOU WISH SPECTRAL DATA? 1=YES;2=NO";
4050 INPUT B7
4051 IF B7 > 1 THEN 4062
4052 IF S > 0 THEN 4062
4053 GO SUB 5000
4054 LET C1=Q2
4055 LET C2=C
4056 IF A5 > 1 THEN 4058
4057 LET C2=A6
4058 GO SUB 6100
4059 EOF #1
4060 LET S=1
4062 IF B6 > 1 THEN 4101
4065 IF B5=1 THEN 4101
4070 FOR I=1 TO B5-1 STEP 1
4080 READ A$
4090 NEXT I
4101 FOR I=B5 TO B8 STEP 1
4102 IF B6 > 1 THEN 4120
4103 READ A$
4105 PRINT
4110 PRINT"#";I;"=  ";TAB(11);A$
4115 LET A$=""
4120 IF B7 > 1 THEN 4201
4130 LET G9=I-Q2+1
4150 DREAD#1,G9,N
4153 FOR J=12 TO N(4) STEP 1
4154 IF N(J)=0 THEN 4157
4155 LET N(J)=N(J))/(100)
4157 NEXT J
4165 PRINT
4170 PRINT"THE SPECTRUM FOR ENTRY NO. ";I;" IS GIVEN BY:"
4175 PRINT
4180 FOR J=12 TO 992 STEP 7
4185 IF J > N(4) THEN 4201
4190 PRINT J;TAB(5);N(J);TAB(13);N(J+1);TAB(23);N(J+2);TAB(31);N(J+3);
4191 PRINT TAB(39);N(J+4);TAB(47);N(J+5);TAB(56);N(J+6)
4200 NEXT J
4201 NEXT I
4205 RESTORE
4210 PRINT"DO YOU WISH FURTHER OUTPUT AT THIS TIME? 1=YES;2=NO";
4220 INPUT D4
4230 IF D4 < 2 THEN 4000
4340 RETURN
5000 LET B$="      "
5010 LET E$="0000"
5016 LET Q3=Q1*100
5020 FOR I=1 TO Q3 STEP 1
5025 READ A$
5030 IF A$(0,2) <> E$ THEN 5050
5035 LET B=I
5040 LET C=I-1
5045 GO TO 5205
5050 IF A$(0,6)=B$ THEN 5140
5060 NEXT I
5065 LET B=Q3+1
5066 LET C=Q3
5080 PRINT"ALL";Q3;"NAME DATA SPACES HAVE BEEN ALLOCATED SO REDEF'N"
```

## APPENDIX I

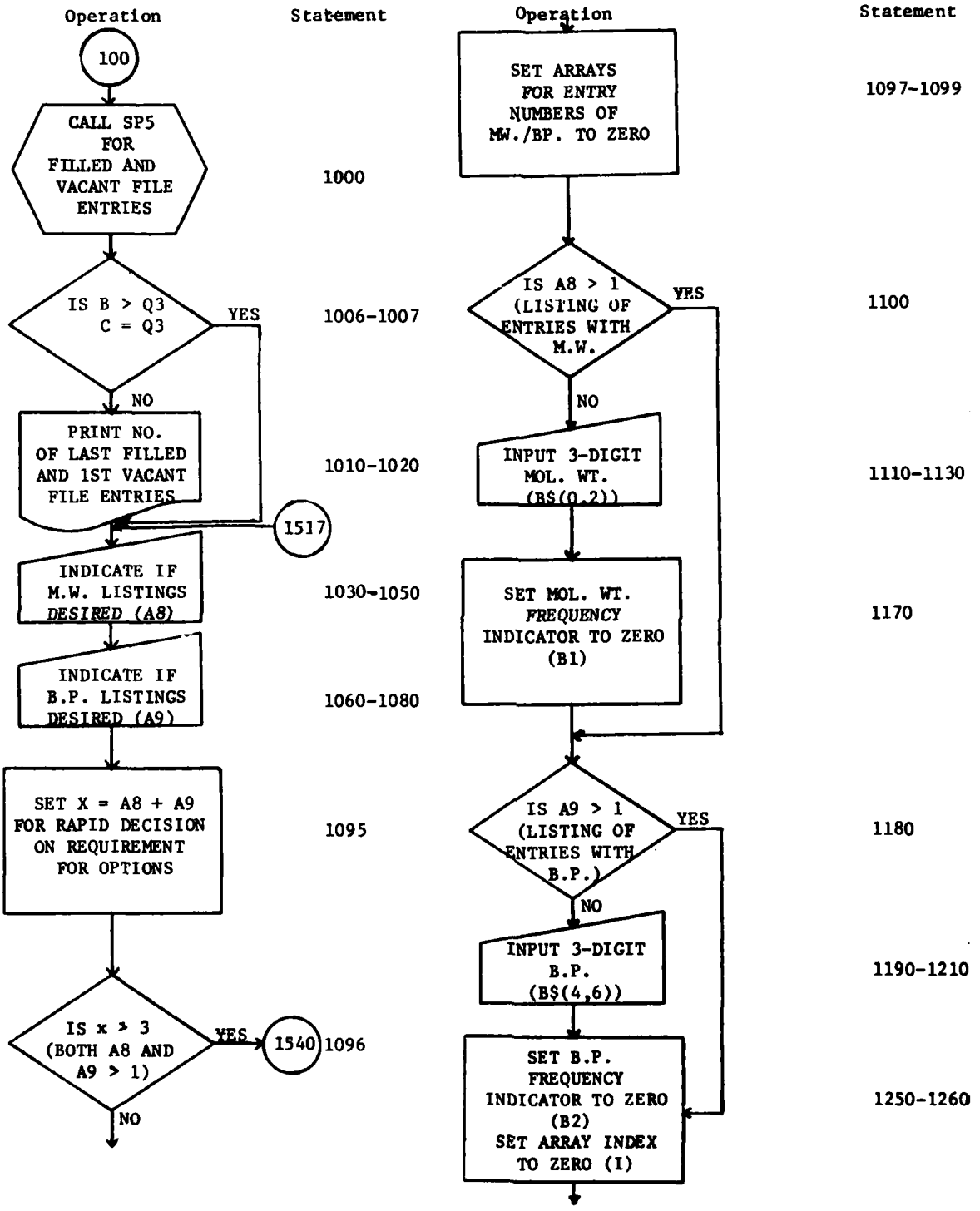
## PROGRAM LISTING - SPECFL

```
5090 PRINT"WILL BE NECESSARY IN THE ENTRY # STATEMENT UNLESS DELETION"
5091 PRINT"IS DESIRED"
5100 PRINT"THE FIRST EMPTY SPACE IS GREATER THAN #";Q3
5130 GO TO 5205
5140 LET B=I
5150 LET C=I-1
5160 FOR J=(B+1) TO Q3 STEP 1
5170 READ A$
5175 IF A$(Ø,2)=E$ THEN 5205
5180 IF A$(Ø,6)=B$ THEN 5200
5190 LET C=J
5200 NEXT J
5205 RESTORE
5210 RETURN
6000 LET H=Ø
6005 FOR J=12 TO 999
6007 IF N(J)=Ø THEN 6025
6009 LET N(4)=J
6010 IF N(J)<=H THEN 6025
6015 LET H=N(J)
6020 LET N(2)=J
6025 NEXT J
6035 PRINT"THE BASE PEAK OCCURS AT";N(2);"AND HIGHEST M/E IS AT";N(4)
6050 FOR I=12 TO N(4)
6060 LET N(I)=((N(I))/(H))*1ØØØØ
6070 NEXT I
6080 RETURN
6100 IF C1>Q2 THEN 6109
6101 FOR I=Ø TO 99Ø STEP 1Ø
6102 LET N(I)=N(I+1)=N(I+2)=N(I+3)=N(I+4)=N(I+5)=Ø
6103 LET N(I+6)=N(I+7)=N(I+8)=N(I+9)=Ø
6104 NEXT I
6105 LET D$="FILE OF INDIVIDUAL SPECTRA
6106 DWRITE #1,D$,N
6109 IF C2<C1 THEN 6220
6110 FOR I=C1 TO C2 STEP 1
6111 LET T=I+1
6126 FOR J=Ø TO 1ØØØ STEP 1
6127 CREAD #T,N(J)
6128 NEXT J
6130 DWRITE #1,D$,N
6140 NEXT I
6220 RETURN
9994 DATA"ØØØ ØØØ"
9995 PRINT"THE PROGRAM IS FINISHED BUT TRANSFER FROM MEMORY TO BASIC"
9996 PRINT"TAPE IS NECESSARY: THE PROGRAM MUST BE STORED UNDER A NEW"
9997 PRINT"NAME TO SAVE CHANGES IN THE ALPHA TEXT"
9998 STOP
9999 END
```

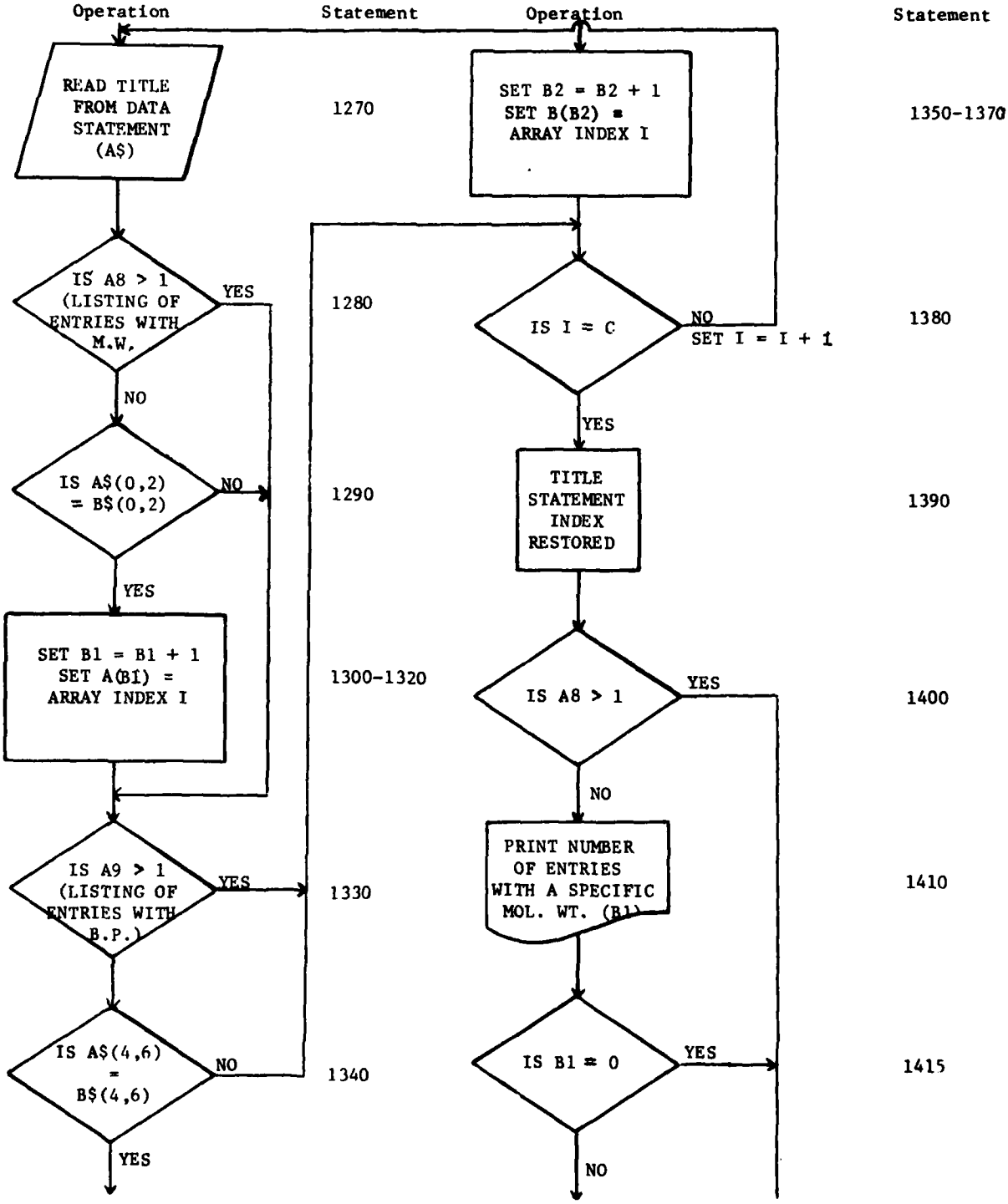
FLOW CHART - MAIN BODY



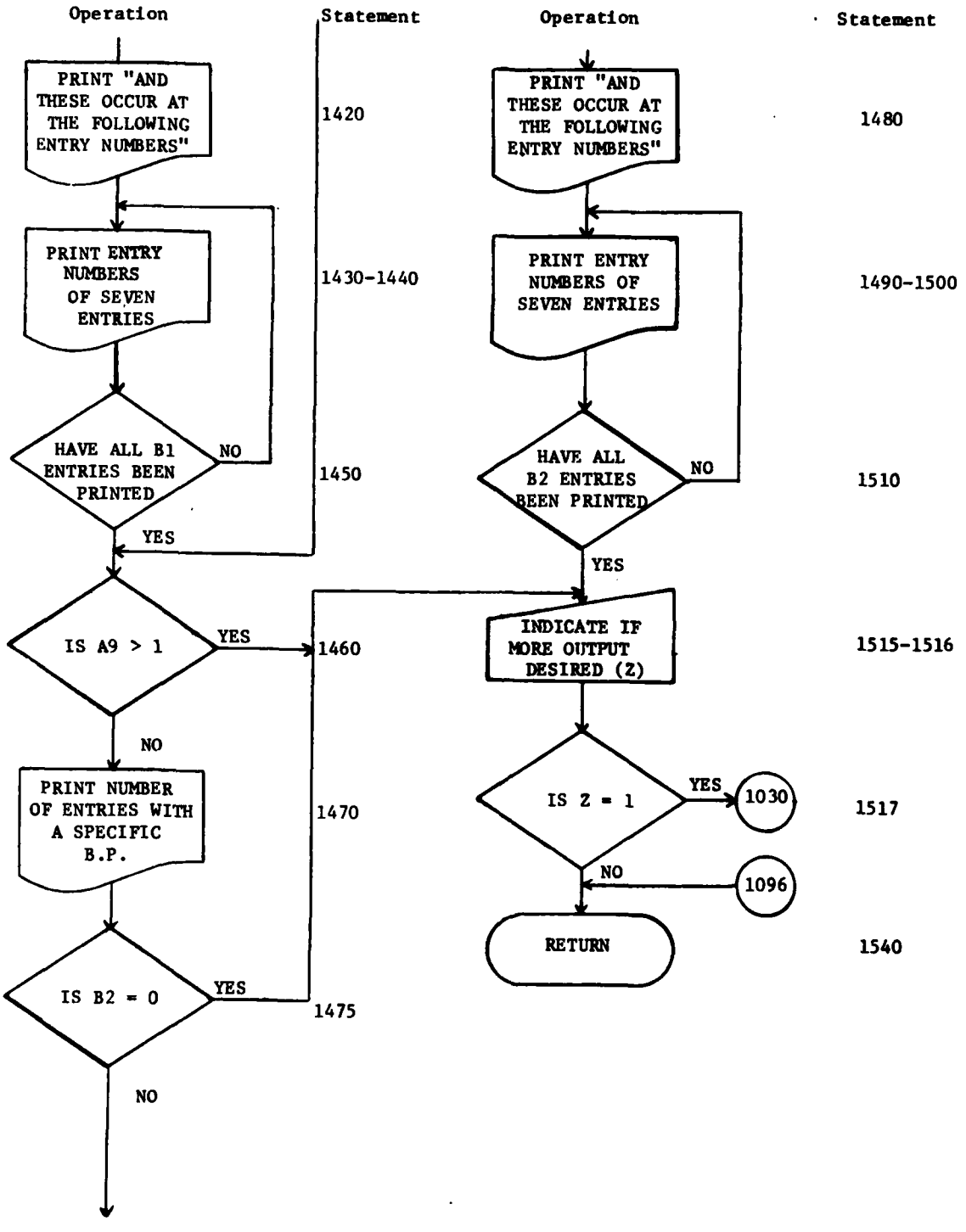
FLOW CHART - SUBPROGRAM 1



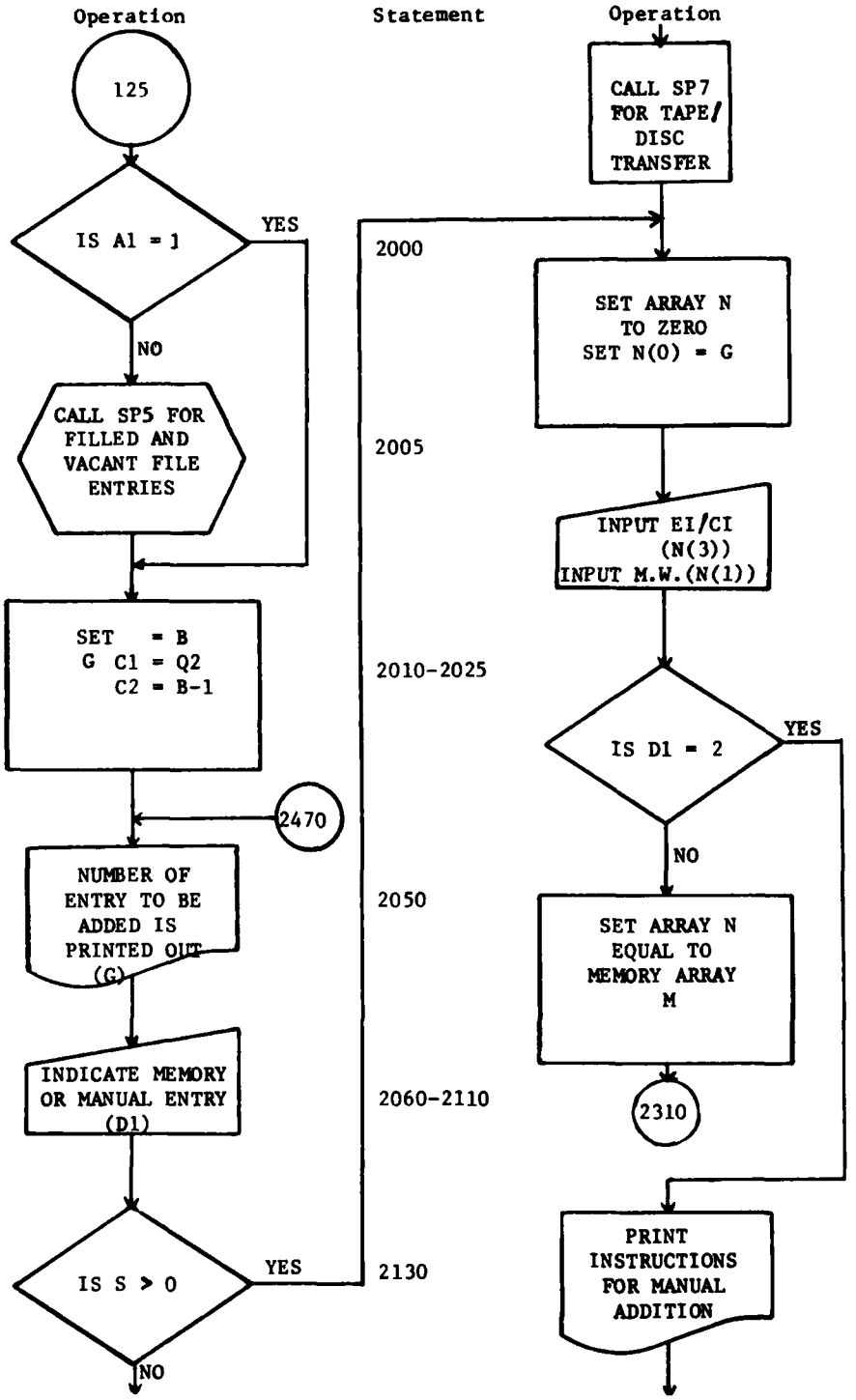
FLOW CHART - SUBPROGRAM 1



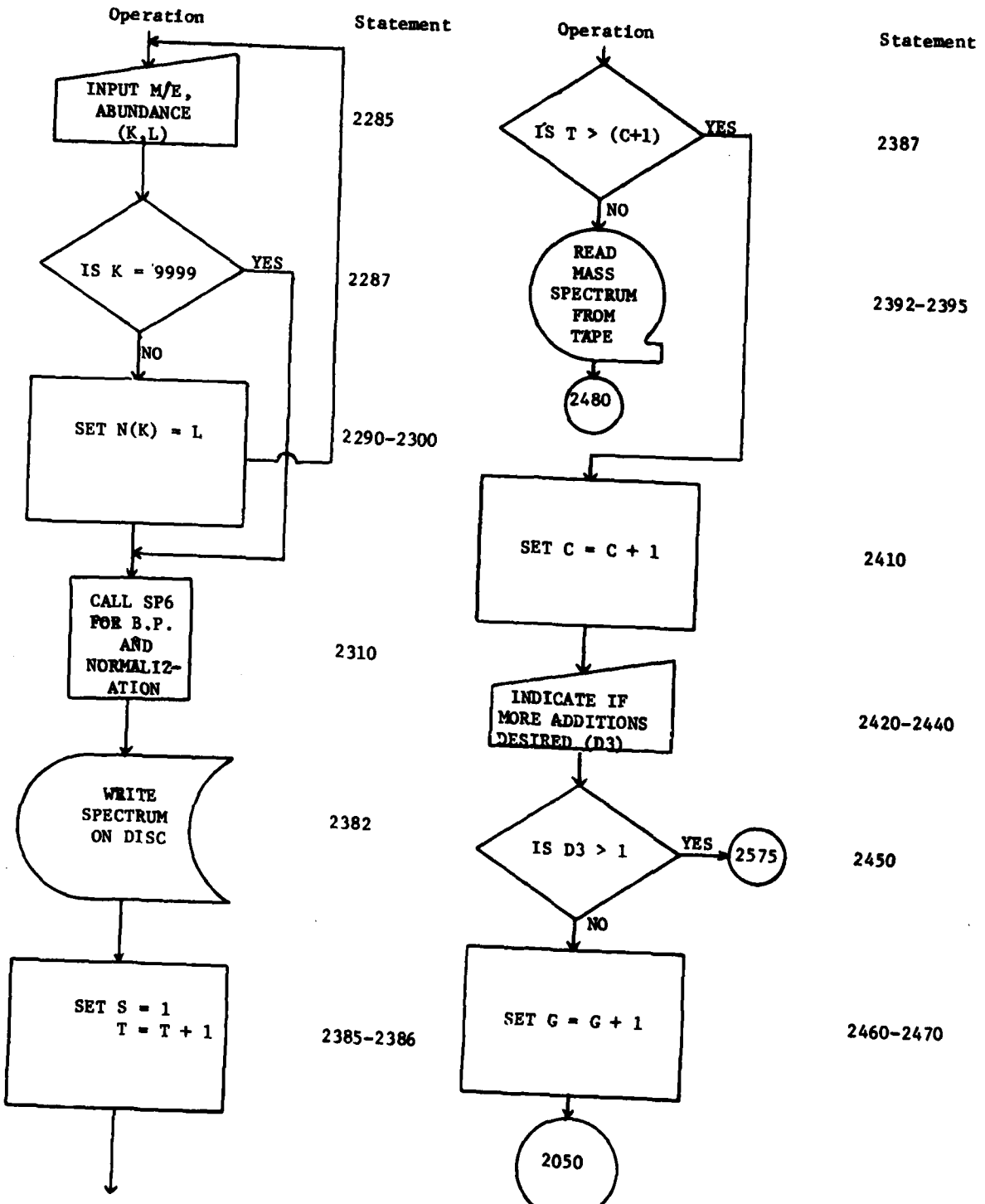
FLOW CHART - SUBPROGRAM 1



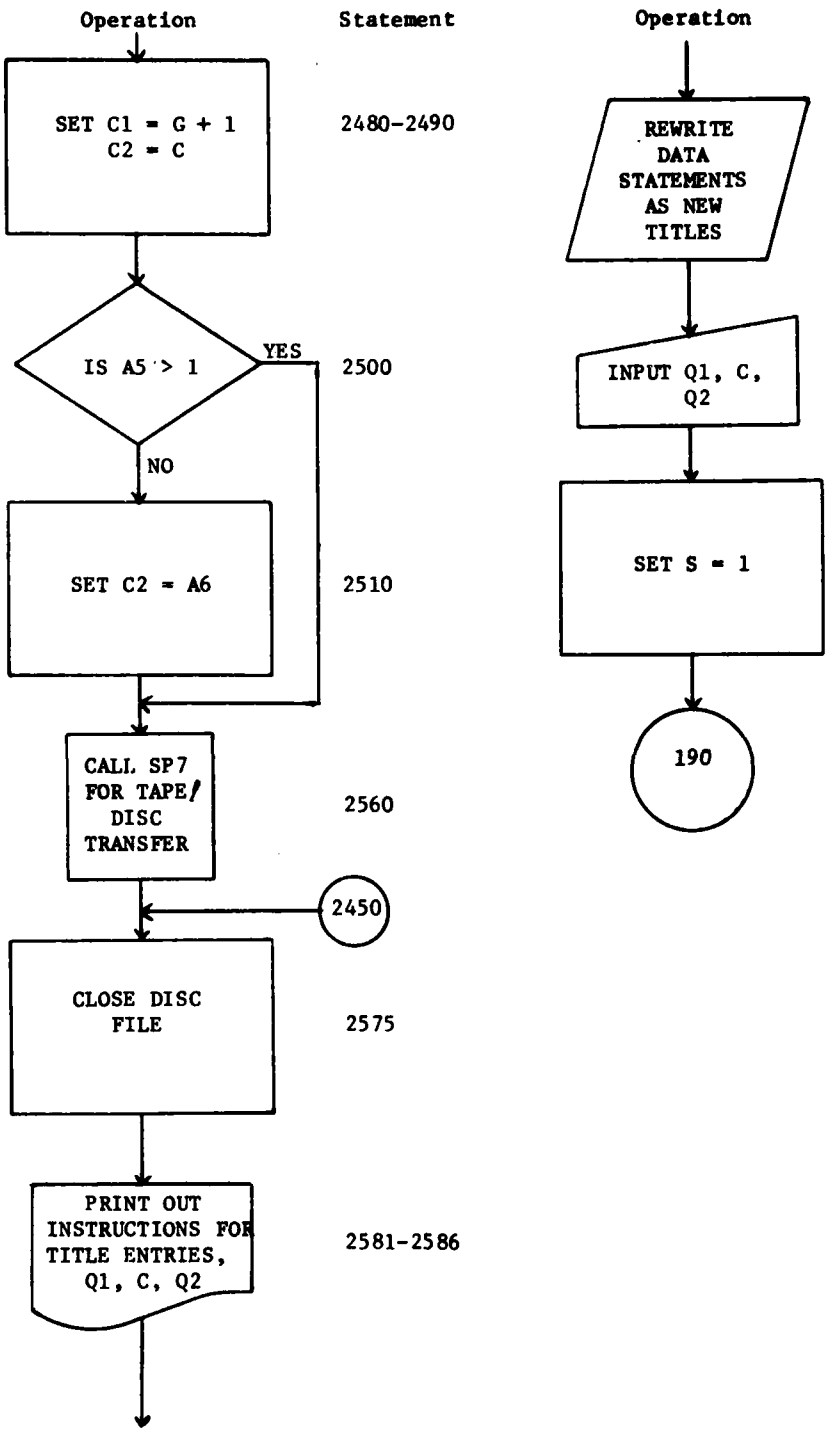
FLOW CHART - SUBPROGRAM 2



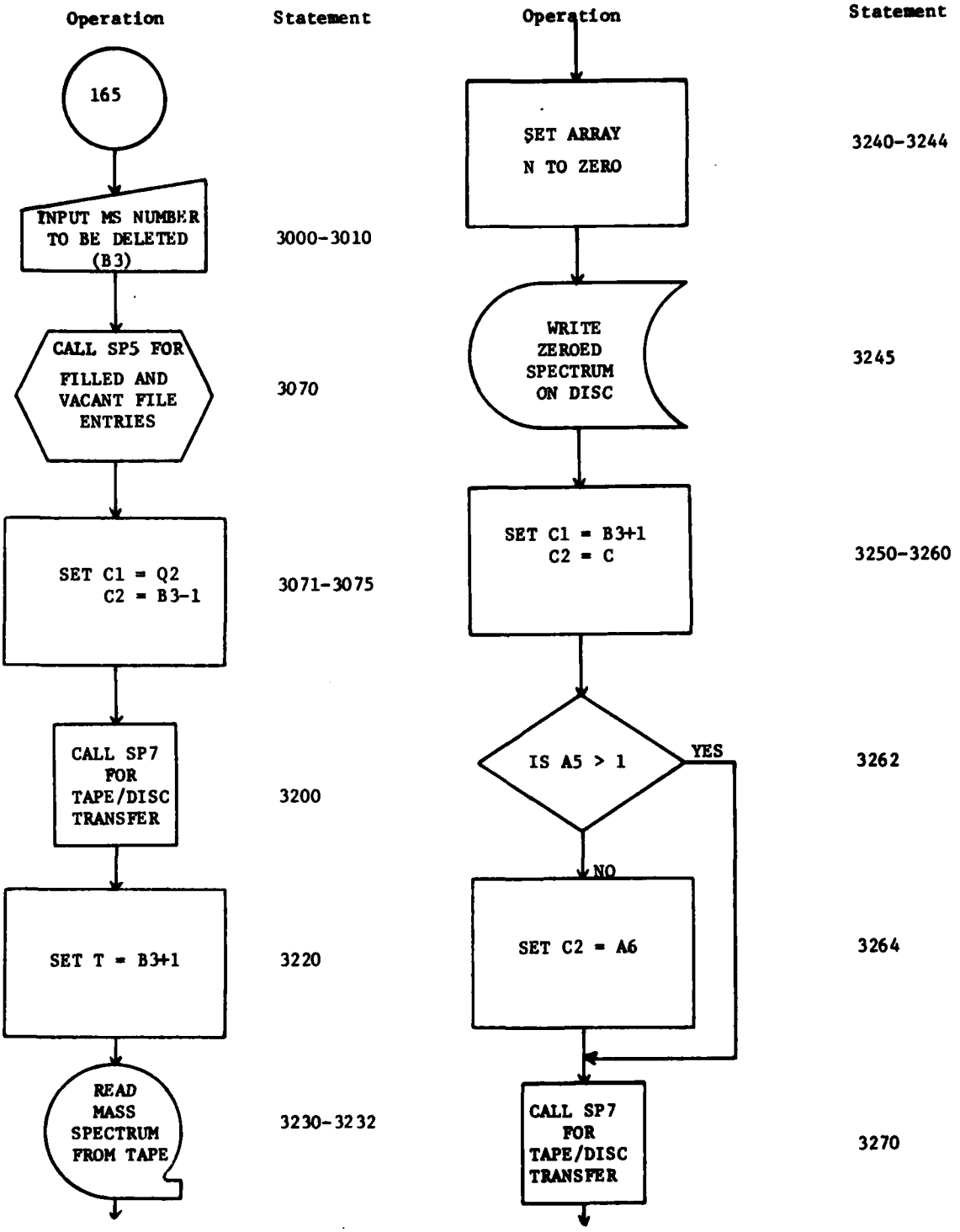
FLOW CHART - SUBPROGRAM 2



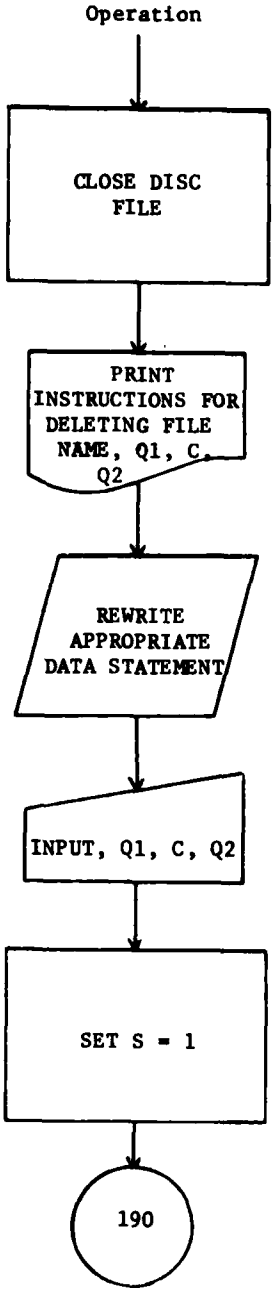
FLOW CHART - SUBPROGRAM 2



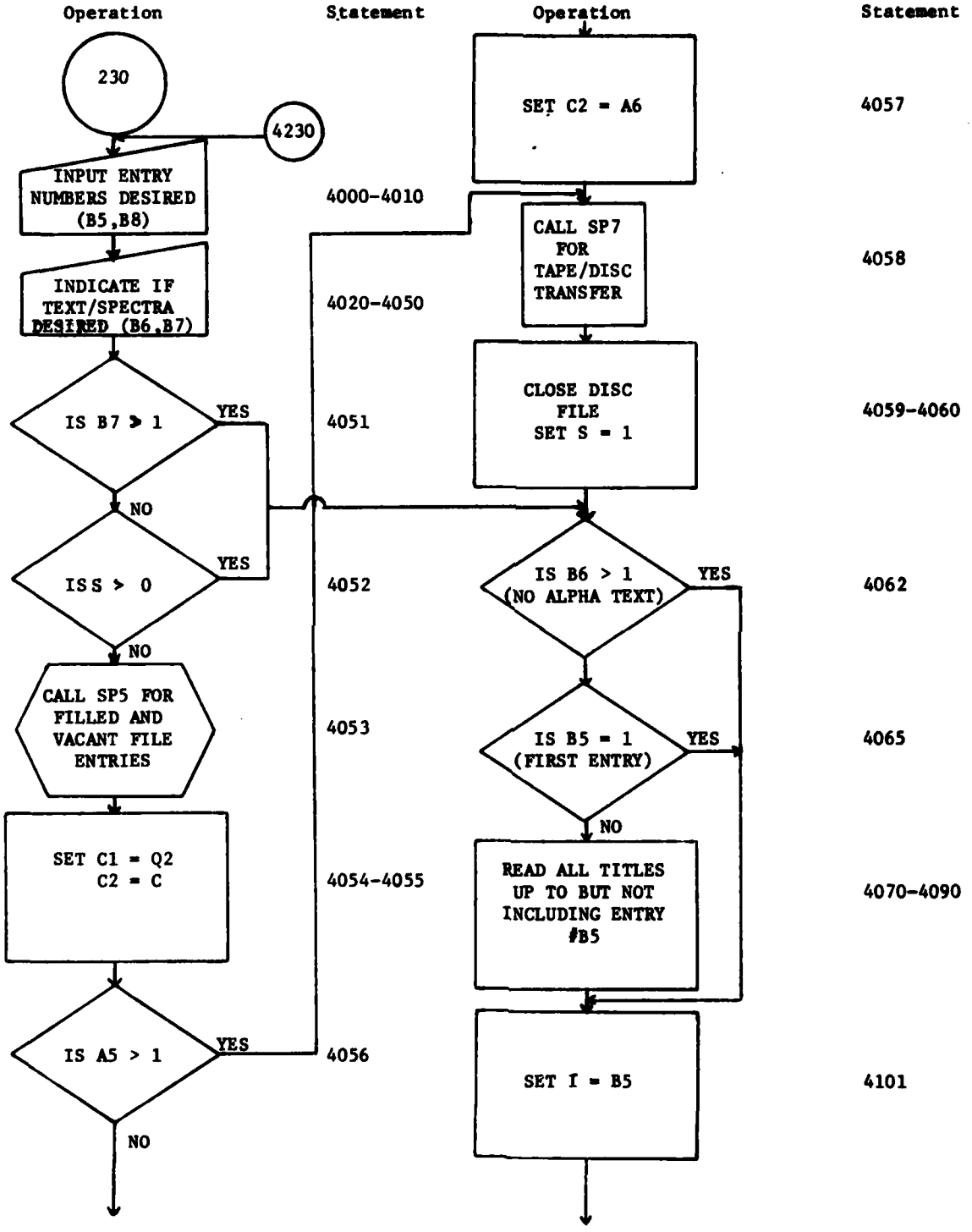
FLOW CHART - SUBPROGRAM 3



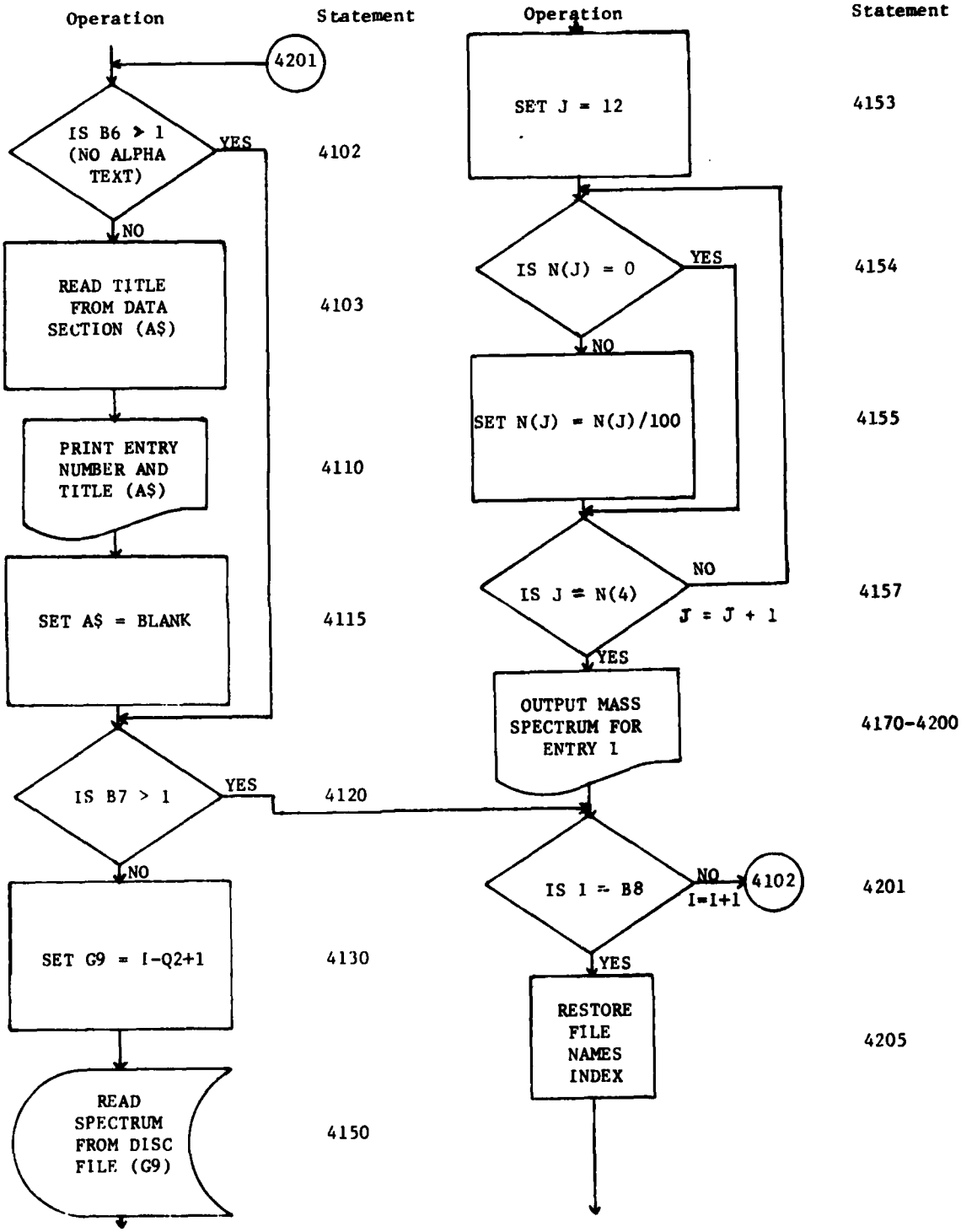
FLOW CHART - SUBPROGRAM 3



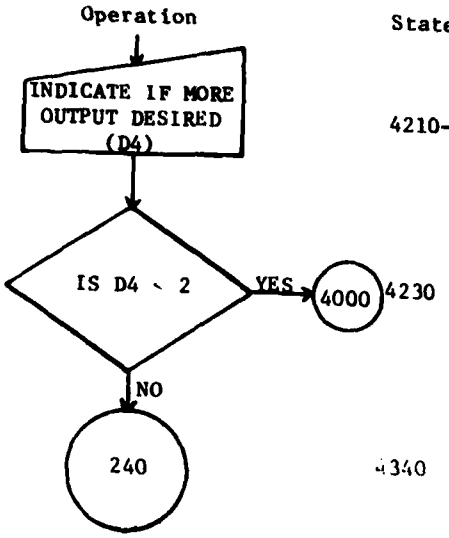
FLOW CHART - SUBPROGRAM 4



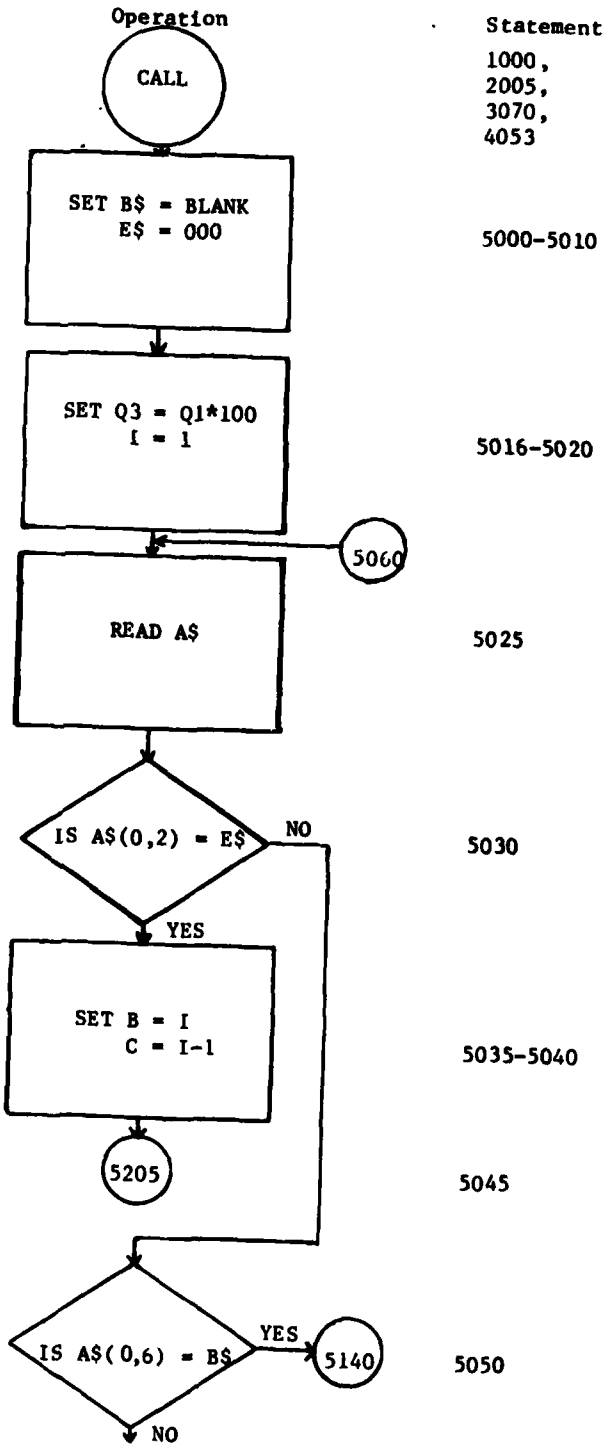
FLOW CHART - SUBPROGRAM 4



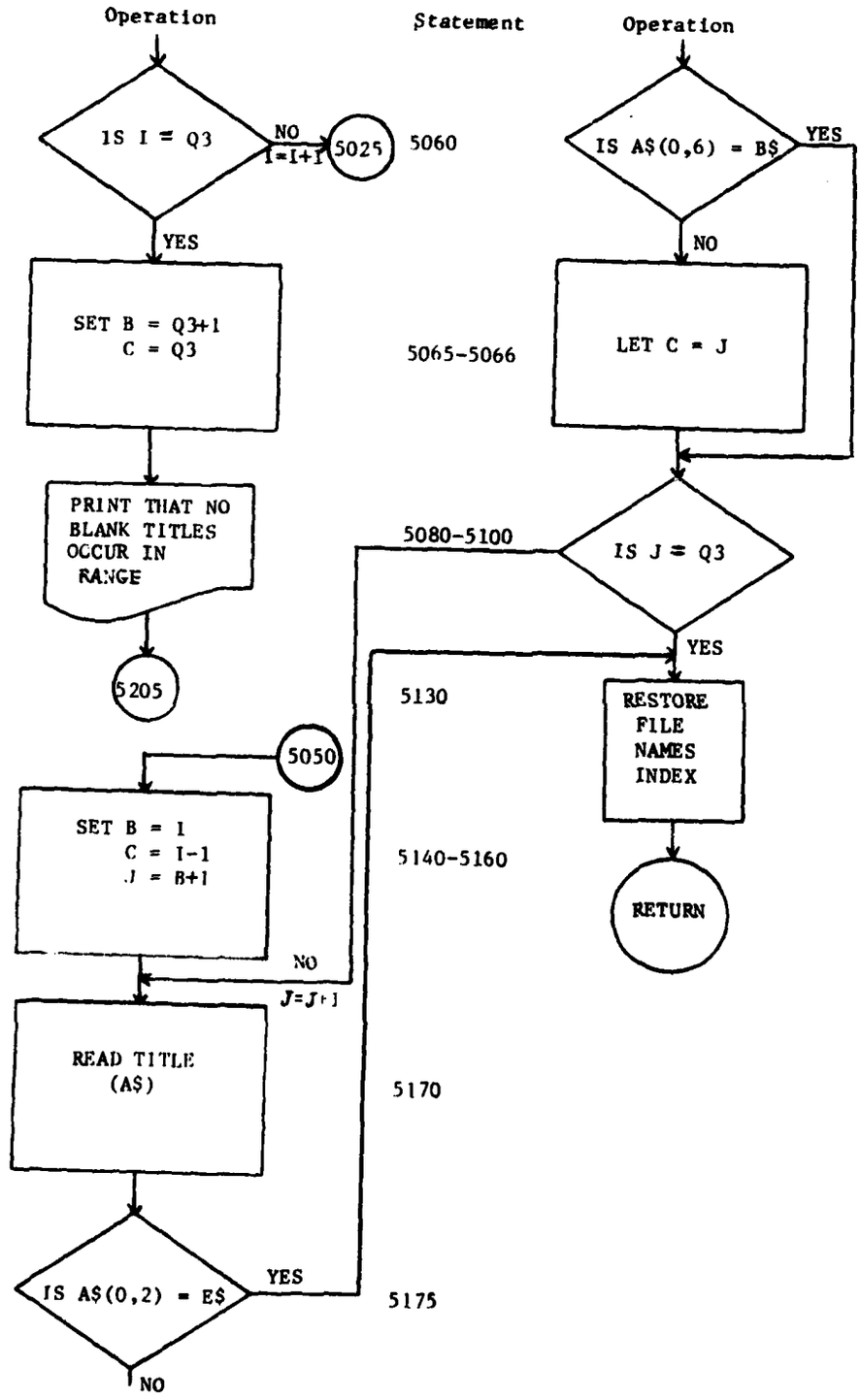
FLOW CHART - SUBPROGRAM 4



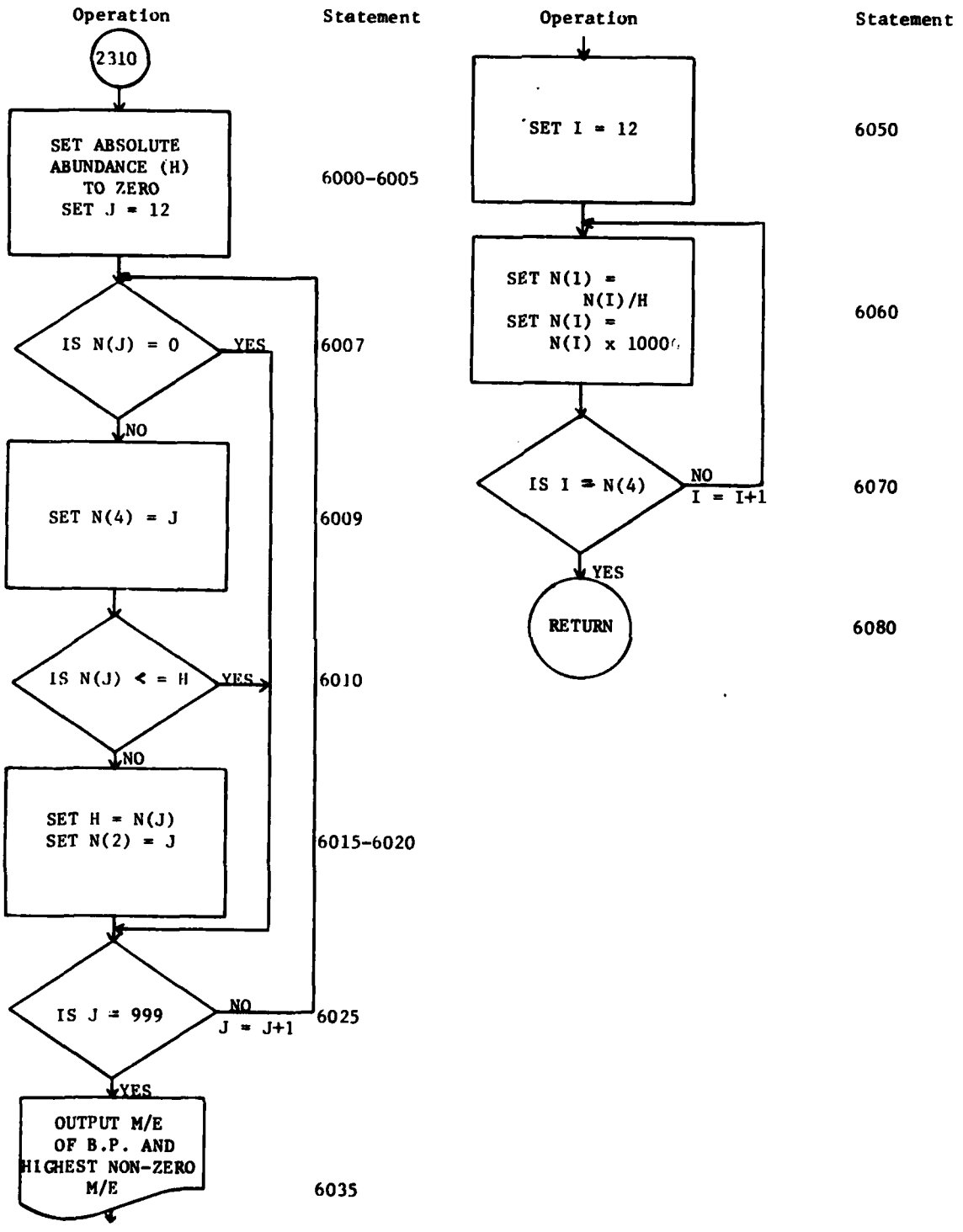

SUBPROGRAM 5



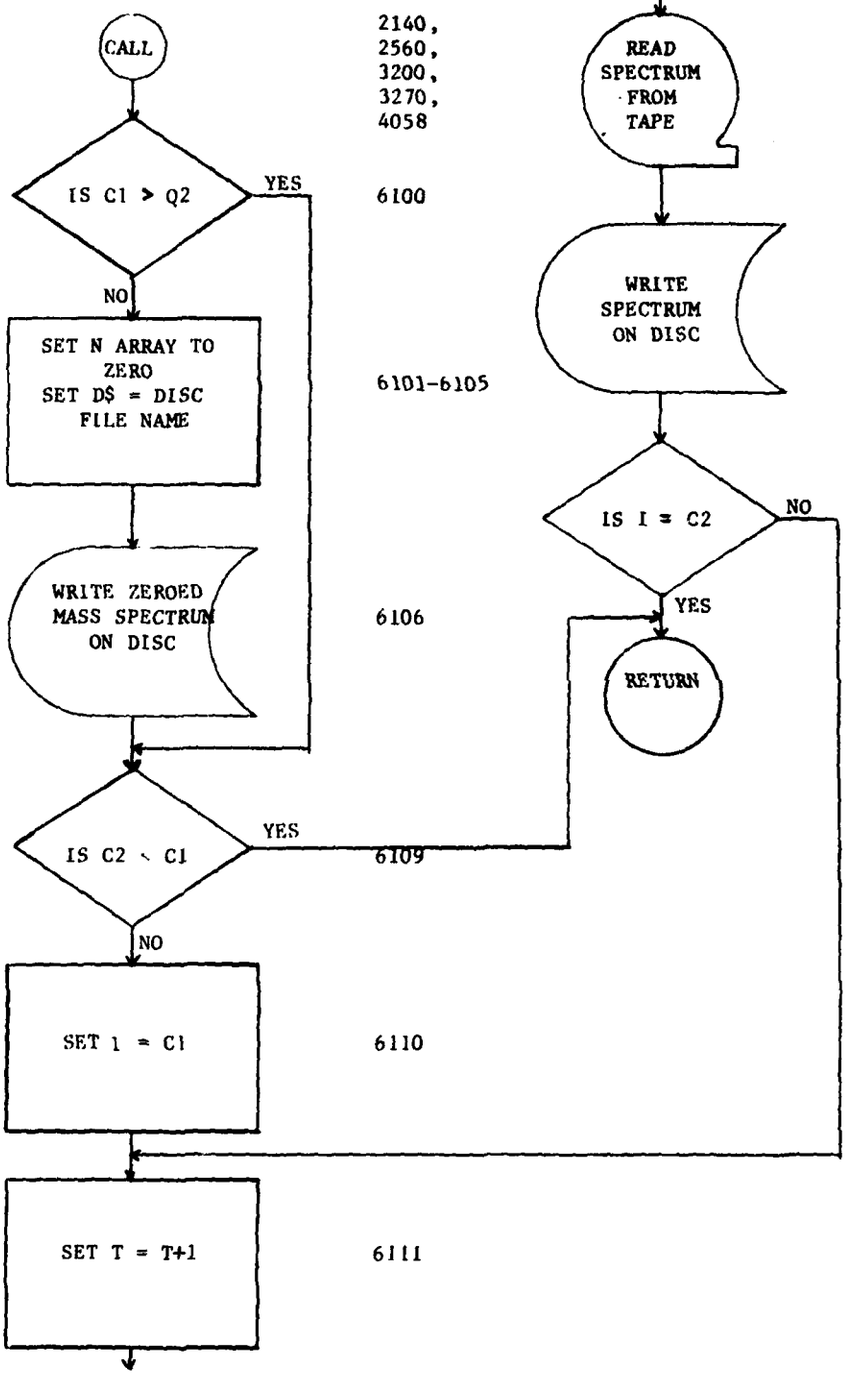
FLOW CHART - SUBPROGRAM 5



FLOW CHART - SUBPROGRAM 6



FLOW CHART - SUBPROGRAM 7



## APPENDIX II

### VARIABLE GLOSSARY - DTRDFN

| | |
|---|---|
| N(I) | A one-dimensional array containing ion abundances for m/e of 12-999 of a mass spectrum and other special information for N(0) - N(11) and N(1000). |
| C,D | Variables to indicate range of mass spectral entries to be transferred. |
| E | Variable to indicate entry number of first spectrum stored in the disc file. |
| K | Variable used to maintain coorelation between entry numbers and disc spectrum numbers. |
| T | Variable used for storage or assignment of tape file names. |

### VARIABLE INDEX - DTRDFN

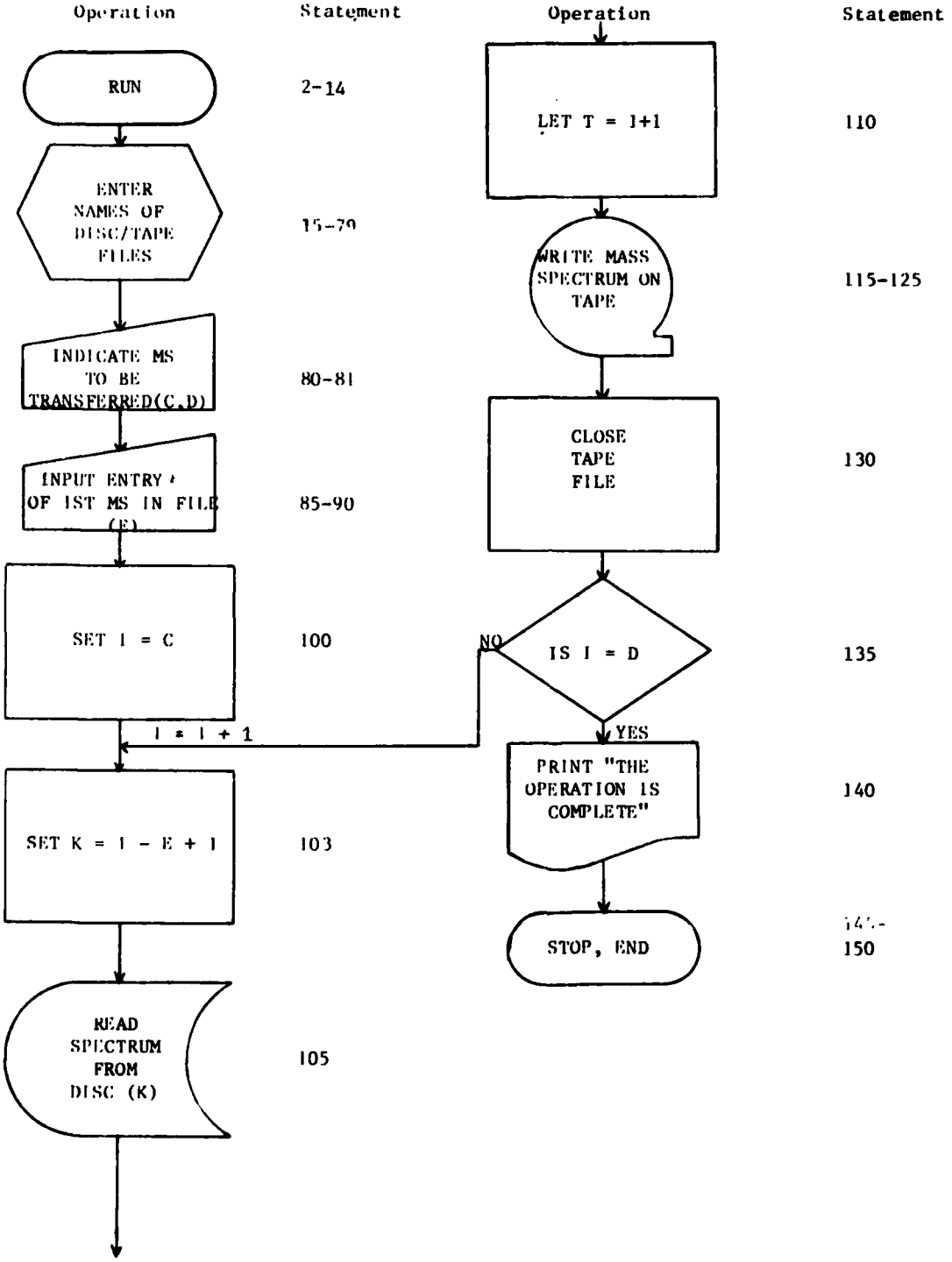
| Variable | Statement No. |
|---|---|
| N(I) | 10,105,120 |
| C | 81,100 |
| D | 81,100 |
| E | 90,103 |
| K | 103,105 |
| T | 110,120,130 |

## APPENDIX I

### PROGRAM LISTING - DTRDFN

```
5    REM THIS PROGRAM READS A SPECTRAL FILE FROM DISC TO TAPE
10   DIM N(1ØØ1)
11   PRINT "ENTER THE NAME OF THE DATA FILE ON THE DISC"
12   PRINT "AS FOLLOWS: 15 FILES NAME"
13   PRINT "THEN TYPE 'GO TO 15'"
14   STOP
15   FILES DISCØØ
16   FILES 1,2,3,4,5,6,7,8,9,1Ø,11,12,13,14,15,16,17,18,19,2Ø,21,22,23,24
17   FILES 25,26,27,28,29,3Ø,31,32,33,34,35,36,37,38,39,4Ø,41,42,43,44,45
18   FILES 46,47,48,49,5Ø,51,52,53,54,55,56,57,58,59,6Ø,61,62,63,64,65,66
19   FILES 67,68,69,70,71,72,73,74,75,76,77,78,79,80,81,82,83,84,85,86,87
20   FILES 88,89,9Ø,91,92,93,94,95,96,97,98,99,1ØØ
80   PRINT"THE ENTRY LIMITS OF SPECTRA TO BE TRANSFERRED ARE";
81    INPUT C,D
85   PRINT"THE ENTRY NUMBER OF 1ST SPECTRUM ON FILE IS";
90   INPUT E
100  FOR I=C TO D STEP 1
103  LET K=I-E+1
105  DREAD #1,K,N
110  LET T=I+1
115  FOR J=Ø T.) 1ØØØ STEP 1
120  CWRITE #T,N(J)
125  NEXT J
130  EOF#T
135  NEXT I
140  PRINT"THE OPERATION IS COMPLETE"
145  STOP
150  END
```

FLOW CHART - DTRDFN



## APPENDIX III

### VARIABLE GLOSSARY - DISCFL

| | |
|---|---|
| A$(I) | - A one-dimensional array for storage of title information of the disc files. |
| N(I) | - A one-dimensional array containing ion abundances for m/e of 12-999 of a mass spectrum and other special information for N(0)-N(9) and N(1000). |
| A | - Variable to indicate number of source disc files to be merged into one composite file. |
| B | - Variable to indicate the first spectrum to be read from a particular disc file*. |
| C | - Variable to indicate the last spectrum to be read from a particular disc file*. |
| M | - Variable to identify disc file to be read. |

### VARIABLE INDEX - DISCFL

| Variable | Statement No. |
|---|---|
| A$(I) | 10,70,80,170 |
| N(I) | 10,30,40,60,80,160,170 |
| A | 100,110 |
| B | 140,150 |
| C | 140,150 |
| M | 120,160 |

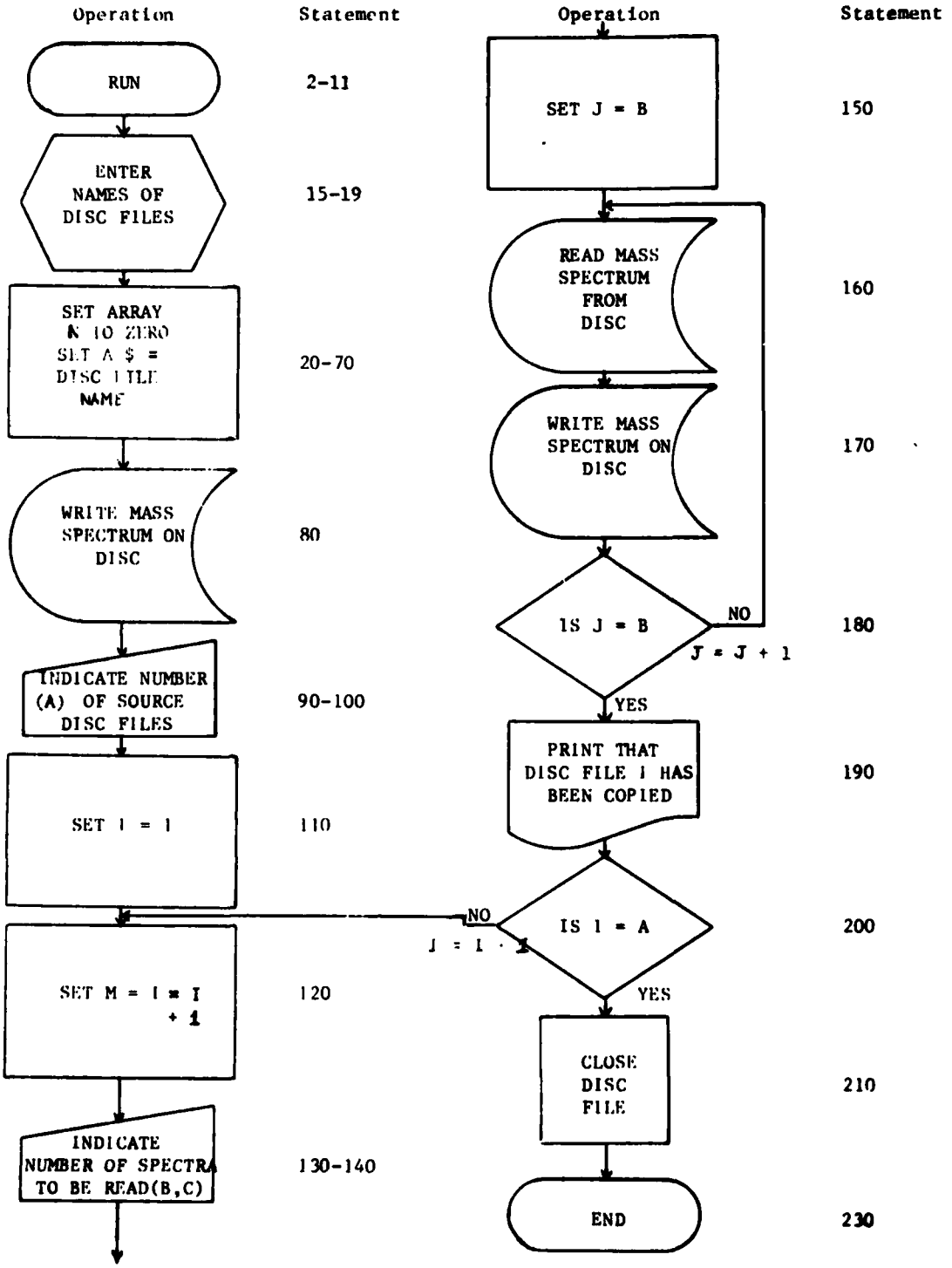
* Every disc file will have spectra starting at position or scan #1 even if the spectrum is entry #201.

## APPENDIX I

## PROGRAM LISTING - DISCFL

```
4    REM THIS PROGRAM CAN MERGE SEVERAL DISC FILES INTO ONE CONSECUTIVE
5    REM FILE ON DISC
6    PRINT"FILES STATEMENTS FOR DISC FILES MUST BE ENTERED AS--15 FILES";
7    PRINT "DISC"
8    PRINT"16 FILES DISCØ1,DISCØ2,DISCØ3,ETC FOR SOURCE FILES, THEN TYPE-";
9    PRINT"GO TO 15-"
10   DIM N(1ØØ1),A$(48)
11   STOP
15   FILES MASØØØ
16   FILES DATA1Ø,MTØØØ2,DATA25
20   FOR I=Ø TO 99Ø STEP 1Ø
30   LET N(I)=N(I+1)=N(I+2)=N(I+3)=N(I+4)=N(I+5)=N(I+6)=N(I+7)=N(I+8)=Ø
40   LET N(I+9)=Ø
50   NEXT I
60   LET N(1ØØØ)=Ø
70   LET A$="FILE OF INDIVIDUAL SPECTRA"
80   DWRITE #1,A$,N
90   PRINT"THE NUMBER OF DISC FILES TO BE READ ARE";
100  INPUT A
110  FOR I=1 TO A STEP 1
120  LET M=I+1
130  PRINT"THE SPECTRA TO BE TRANSFERRED IN FILE #";I;"ARE";
140  INPUT B,C
150  FOR J=B TO C STEP 1
160  DREAD #M,J,N
170  DWRITE #1,A$,N
180  NEXT J
190  PRINT"DISC FILE #";I;"HAS BEEN COPIED"
200  NEXT I
210  EOF #1
220  STOP
230  END
```

FLOW CHART - DISCFL



## APPENDIX IV

### VARIABLE GLOSSARY - TRANTD

| | |
|---|---|
| A$(I) | - A one-dimensional array for storage of title information of the disc file. |
| N(I) | - (as in Appendix III) |
| P | - Variable to indicate entry number of first mass spectrum to be transferred. |
| R | - Variable to indicate entry number of last mass spectrum to be transferred. |
| T | - Variable to identify tape file to be read. |

### VARIABLE INDEX - TRANTD

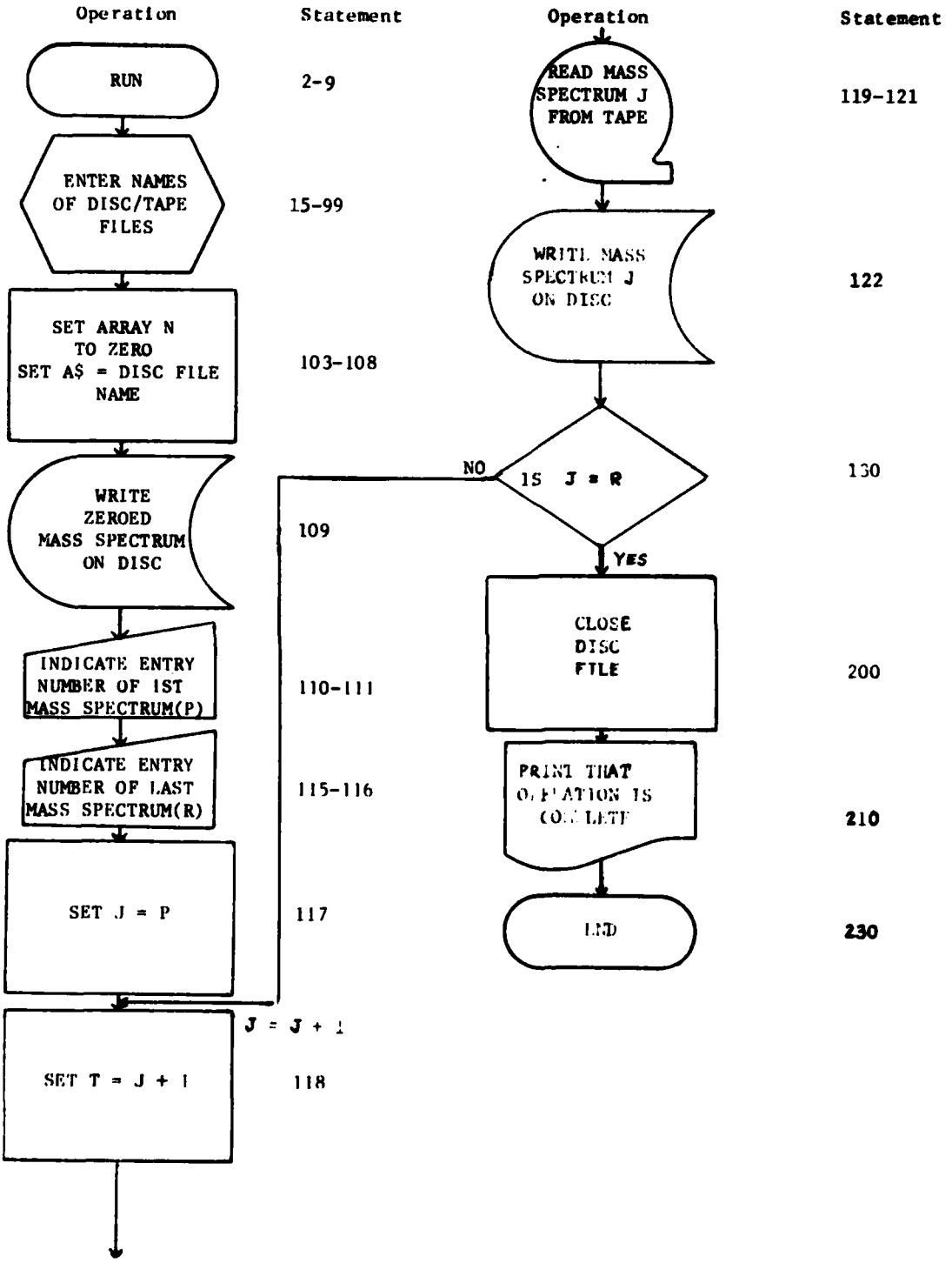
| Variable | Statement No. |
|---|---|
| A$(I) | - 100,108,109,122 |
| N(I) | - 100,104,105,107,109,120,122 |
| P | - 111,117 |
| R | - 116,117 |
| T | - 118,120 |

## APPENDIX I

### PROGRAM LISTING - TRANTD

```
4     REM THIS PROGRAM CAN TRANSFER SPECTRAL FILES FROM TAPE TO A SINGLE
5     REM FILE ON DISC
6     PRINT"FILES STATEMENTS FOR ALL SPECTRAL FILES MUST BE ENTERED THUS"
7     PRINT"15 FILES DISC-FOR DISC FILE;16 FILES 1,2,3,...ETC. FOR TAPE"
8     PRINT"THEN INSERT SPECTRAL TAPE AND TYPE 'GO TO 15'"
9     STOP
15    FILES DISCØ1
16    FILES 1,2,3,4,5,6,7,8,9,1Ø,11,12,13,14,15,16,17,18,19,2Ø,21,22,23,24
17    FILES 25,26,27,28,29,3Ø,31,32,33,34,35,36,37,38,39,4Ø,41,42,43,44,45
18    FILES 46,47,48,49,5Ø,51,52,53,54,55,56,57,58,59,6Ø,61,62,63,64,65,66
19    FILES 67,68,69,7Ø,71,72,73,74,75,76,77,78,79,8Ø,81,82,83,84,85,86,87
20    FILES 88,89,9Ø,91,92,93,94,95,96,97,98,99,1ØØ,1Ø1,1Ø2,1Ø3,1Ø4,1Ø5,1Ø6
100   DIM N(1ØØ1),A$(48)
103   FOR I=Ø TO 99Ø STEP 1Ø
104   LET N(I)=N(I+1)=N(I+2)=N(I+3)=N(I+4)=N(I+5)=N(I+6)=N(I+7)=Ø
105   LET N(I+8)=N(I+9)=Ø
106   NEXT I
107   LET N(1ØØØ)=Ø
108   LET A$="FILE OF INDIVIDUAL SPECTRA"
109   DWRITE #1,A$,N
110   PRINT"INPUT ENTRY # FOR FIRST MS TO BE TRANSFERRED";
111   INPUT P
115   PRINT"INPUT ENTRY # OF LAST MS TO BE TRANSFERRED";
116   INPUT R
117   FOR J=P TO R STEP 1
118   LET T=J+1
119   FOR I=Ø TO 1ØØØ STEP 1
120   CREAD #T,N(I)
121   NEXT I
122   DWRITE #1,A$,N
130   NEXT J
200   EOF #1
210   PRINT "THE OPERATION IS COMPLETE"
220   STOP
230   END
```

FLOW CHART - TRANTD



UNCLASSIFIED

Security Classification

## DOCUMENT CONTROL DATA - R & D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall document is classified)

| | |
|---|---|
| ORIGINATING ACTIVITY<br>Defence Research Establishment Ottawa | 2a. DOCUMENT SECURITY CLASSIFICATION<br>Unclassified<br>2b. GROUP |

3. DOCUMENT TITLE
**Finnigan BASIC Computer Programs for the Entry, Display and Compact Storage of Mass Spectra in a Finnigan 6115 Data System**

4. DESCRIPTIVE NOTES (Type of report and inclusive dates)
Technical Note

5. AUTHOR(S) (Last name, first name, middle initial)
Purdon, J. Garfield

| | | |
|---|---|---|
| 6. DOCUMENT DATE<br>March 1981 | 7a. TOTAL NO. OF PAGES<br>44 | 7b. NO. OF REFS<br>1 |
| 8a. PROJECT OR GRANT NO | 9a. ORIGINATOR'S DOCUMENT NUMBER(S)<br>DREO Technical Note 82-2 | |
| 8b. CONTRACT NO | 9b. OTHER DOCUMENT NO.(S) (Any other numbers that may be assigned this document) | |

10. DISTRIBUTION STATEMENT
Unlimited distribution

| | |
|---|---|
| 11. SUPPLEMENTARY NOTES | 12. SPONSORING ACTIVITY |

13. ABSTRACT

Finnigan BASIC programs have been developed for the creation, compact storage and output of files containing mass spectra on a Finnigan 6115 Data system used with Finnigan 3000 and 4000 Series Gas Chromatograph/Mass Spectrometers. Entries can be made directly from the memory of the data system for spectra acquired on the specific instrument or from a keyboard for spectra obtained from external compilations. The resulting mass spectra can be stored both in Finnigan BASIC or magnetic tape permitting further BASIC operations and or magnetic disc in the computer for standard mass spectral manipulation by the operating system.

DD FORM 1473 (04-81)

Security Classification

**KEY WORDS**

Mass Spectral Data Storage
BASIC computer program

**INSTRUCTIONS**

1. ORIGINATING ACTIVITY: Enter the name and address of the organization issuing the document.

2a. DOCUMENT SECURITY CLASSIFICATION: Enter the overall security classification of the document including special warning terms whenever applicable.

2b. GROUP: Enter security reclassification group number. The three groups are defined in Appendix 'M' of the DRB Security Regulations.

3. DOCUMENT TITLE: Enter the complete document title in all capital letters. Titles in all cases should be unclassified. If a sufficiently descriptive title cannot be selected without classification, show title classification with the usual one-capital-letter abbreviation in parentheses immediately following the title.

4 DESCRIPTIVE NOTES: Enter the category of document, e.g. technical report, technical note or technical letter. If appropriate, enter the type of document, e.g. interim, progress, summary, annual or final. Give the inclusive dates when a specific reporting period is covered.

5 AUTHOR(S): Enter the name(s) of author(s) as shown on or in the document. Enter last name, first name, middle initial. If military, show rank. The name of the principal author is an absolute minimum requirement.

6 DOCUMENT DATE: Enter the date (month, year) of Establishment approval for publication of the document.

7a. TOTAL NUMBER OF PAGES: The total page count should follow normal pagination procedures, i.e., enter the number of pages containing information.

7b. NUMBER OF REFERENCES: Enter the total number of references cited in the document.

8a PROJECT OR GRANT NUMBER: If appropriate, enter the applicable research and development project or grant number under which the document was written.

8b. CONTRACT NUMBER: If appropriate, enter the applicable number under which the document was written.

9a. ORIGINATOR'S DOCUMENT NUMBER(S): Enter the official document number by which the document will be identified and controlled by the originating activity. This number must be unique to this document.

9b. OTHER DOCUMENT NUMBER(S): If the document has been assigned any other document numbers (either by the originator or by the sponsor), also enter this number(s).

10. DISTRIBUTION STATEMENT: Enter any limitations on further dissemination of the document, other than those imposed by security classification, using standard statements such as:

(1) "Qualified requesters may obtain copies of this document from their defence documentation center."

(2) "Announcement and dissemination of this document is not authorized without prior approval from originating activity."

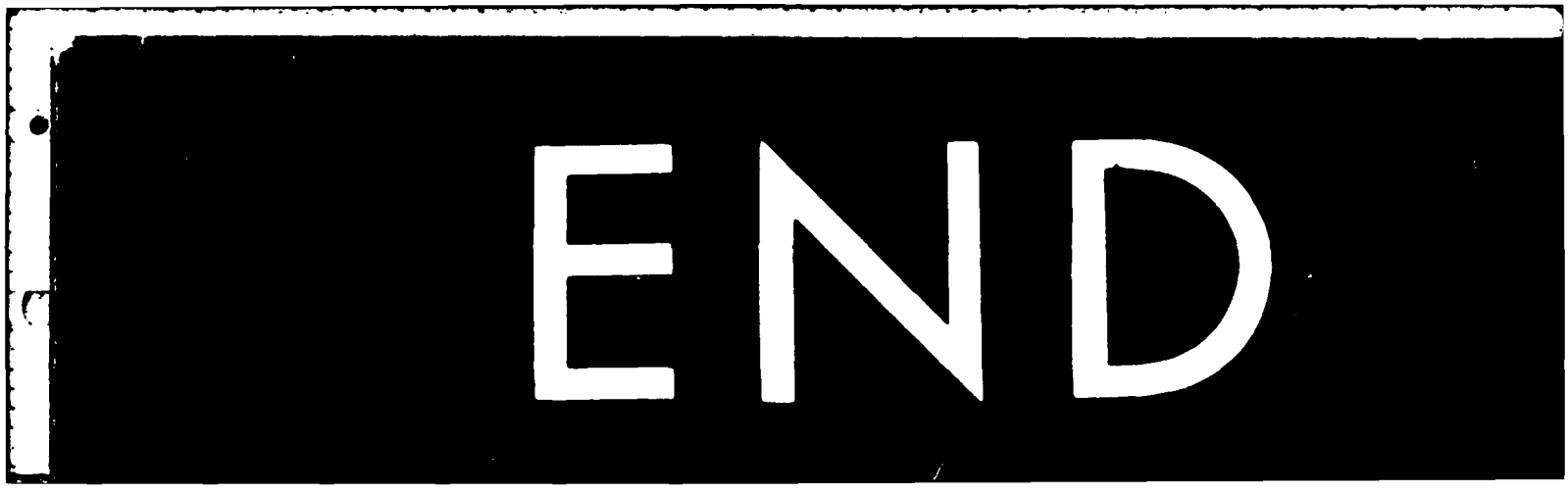
11. SUPPLEMENTARY NOTES: Use for additional explanatory notes.

12. SPONSORING ACTIVITY: Enter the name of the departmental project office or laboratory sponsoring the research and development. Include address.

13. ABSTRACT: Enter an abstract giving a brief and factual summary of the document, even though it may also appear elsewhere in the body of the document itself. It is highly desirable that the abstract of classified documents be unclassified. Each paragraph of the abstract shall end with an indication of the security classification of the information in the paragraph (unless the document itself is unclassified) represented as (TS), (S), (C), (R), or (U).

The length of the abstract should be limited to 20 single-spaced standard typewritten lines; 7½ inches long.

14. KEY WORDS: Key words are technically meaningful terms or short phrases that characterize a document and could be helpful in cataloging the document. Key words should be selected so that no security classification is required. Identifiers, such as equipment model designation, trade name, military project code name, geographic location, may be used as key words but will be followed by an indication of technical context.


END